The
Mechanics and Thermodynamics
of Continuous Media

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Preface

This book presents the nonlinear theories of continuum thermomechanics. Throughout I emphasize issues that are foundational in nature, and seek results common to materials of arbitrary symmetry. The central part of the book deals with thermoelastic bodies with heat conduction and viscosity, including the inviscid or ideal dissipationless bodies. A surprising variety of phenomena can be modeled within this framework. Moreover, the main ideas can be transferred into more complicated theories.

At present, the major challenge to the nonlinear thermoelasticity is posed by phase transformations with changes in symmetry. J. W. Gibbs' immensely influential treatise *On the equilibrium of heterogeneous substances* has provided a highly successful theory of phase transitions in fluids. Gibbs brought the view that the thermodynamics is not only the theory of heat, but also a theory of equilibrium, with the main tool the minimum principles. A large portion of the book is an extension of Gibbs' ideas to bodies of general symmetry by the methods of the calculus of variations. The interplay between the convexity properties of the stored energy functions, the resulting equations, and the physics of the phenomena is a leading theme.

I would like to thank many people for discussions held over the years of this long-term project, and reserve the chief place among them for Jan Kratochvíl and Ivan Samohýl. Earlier versions were written partly during my stays at the Institute for Mathematics and its Applications, University of Minnesota, Minneapolis, CNUCE, Istituto di C.N.R., Pisa, Helsinki Technological University, Espoo, and at Carnegie Mellon University, Pittsburgh, Pa. The hospitality of these institutions is gratefully acknowledged. Special thanks are due to I. Samohýl, W. Hrusa, and J. Vítek, who read earlier versions and suggested many improvements, and to Professor W. Beiglböck who contributed with valuable remarks. I also gratefully acknowledge the support of Grant No. 119110 of the Academy of Sciences of the Czech Republic during the final stage of the project.

Prague, April 1996 M. Šilhavý

Synopsis

To allow the existence of phase transformations, shock waves and other phenomena, the response of a body must be nonlinear. As this book is designed to treat bodies with a response of general symmetry, the deformation gradient must be used as the basic measure of deformation. The passage to specific symmetries – isotropic solids, fluids, or crystals – is made only to reach conclusions that do not hold generally, or to give the general assertions a more concrete form in the variables of the specific situation. The relationship between the response functions and the material behavior is established by isolating leading features of the response functions rather than by examining concrete models. Apart from the natural restrictions from the entropy inequality, frame indifference, and symmetry, the main unifying concepts are the convexity/nonconvexity properties of the thermodynamic potentials.

The understanding of these concepts is now much fuller than, say, at the time of [Truesdell and Noll, 1965]. Since then, the closely related concepts of quasiconvexity and rank 1 convexity have proved to be basic for the mathematical theory of materials. They are related to the qualitative features of the equilibrium states, like their existence/nonexistence, stability/instability, uniqueness/nonuniqueness, the occurrence/nonoccurrence of phase boundaries, etc. Moreover, the violation of these and other 'mathematically desirable' features is now understood *not* as a mathematical pathology, but as a sign indicating (the possibility of) an interesting physical phenomenon, phase transition, observable large- or fine-scale instability or another 'catastrophic' feature. For fluids, the quasiconvexity and rank 1 convexity in the deformation gradient reduce to the convexity in the specific volume, and its relevance to the stability has been known since the times of Gibbs. Also the violation of the convexity of the energy, i.e., the occurrence of an interval where the pressure increases with the specific volume (the spinodal interval of the Van der Waals isotherm), is clearly necessary for a phase transition. The values of the specific volumes of the stably coexistent liquid and its vapor are determined from the equality of the chemical potentials of the phases.

The quasiconvexity and rank 1 convexity in the deformation gradient are the generalizations of the convexity in the specific volume for fluids, and the continuity of the normal component of the *Eshelby energy-momentum tensor* across the static phase interface is the generalization of the equality of the chemical potentials. The common origin of the quasiconvexity and of the continuity of the Eshelby tensor is in the minimum principles, e.g., the principle of minimum total stored energy. (The past attempts to generalize the convexity on an a priori basis, and the attempts to generalize the equality of chemical potentials by formal considerations, have proved unsuccessful.) At the regions where the rank 1 convexity prevails, the equations of mechanical equilibrium are elliptic. The occurrence of the spinodal region in fluids is translated into the violation of the rank 1 convexity on a subinterval of the line segment connecting the deformation gradients at the two sides of the interface ("generalized spinodal region"). These are unavoidable consequences of minima, valid for the response of a general symmetry, with numerous consequences. The theory of materials in equilibrium appears to be quite mature. Wide varieties of mathematical tools have been assembled, with major profit from and impact on the calculus of variations, partial differential equations and nonlinear functional analysis.

In dynamics, the thermal phenomena cannot be neglected. If the static theory admits states with several coexistent phases, the dynamic theory must describe the evolution of the phase interfaces, and in this respect it may be viewed as a broad generalization of the Stefan problem. Moreover, the energy function cannot be globally elliptic and the evolution equations change their type from hyperbolic to *elliptic* in the spinodal region. A violent nonuniqueness in the initial-value problem accompanies that, a nonuniqueness far more severe than the known nonuniqueness in the hyperbolic systems of nonlinear conservation laws. The results concerning this general approach are scarce. The present book describes a recent proposal for an additional kinetic equation for the speed of an evolving phase boundary. This is another interesting application of the Eshelby tensor.

The idealized dissipationless materials are described in a more detail. The ever-present discontinuities of solutions are shock waves, and the thermodynamics provides the entropy admissibility criterion, i.e., the increase of entropy across the shock. In fluids in the hyperbolic and genuinely nonlinear regimes, the shock waves and the entropy criterion are understood, at least on the constitutive level, since the late forties. The genuine nonlinearity means here that the pressure is a convex function of the specific volume at constant entropy, another remarkable constitutive restriction. The entropy criterion is known to secure the realistic behavior of shocks, most notably the uniqueness in the Riemann problem and Lax' inequalities. When the genuine nonlinearity fails but the hyperbolicity still holds, the entropy criterion is insufficient for that, and Liu's criterion must be employed, which may be interpreted as a strengthening of Lax' inequalities, or as a generalization of Oleinik's E-condition to systems of equations. Its relation to the entropy criterion is established, both for bodies of general material symmetry and for fluids. Naturally, the latter case leads to more perfect results.

Part I deals with the basic language of continuum mechanics. This includes tensor algebra and analysis, the geometry and kinematics of continuous bodies, and the balance equations. The constitutive equations characterizing particular materials are kept distinct form the balance equations, as is now common. The direct notation is used throughout. In the tensor analysis, the emphasis is on somewhat less standard questions like the differentiation of the eigenvalues of the stretch tensors (principal strains) with respect to the deformation gradient, differentiation of the square root of a tensor, etc. The kinematics deliberately avoids the classical analysis of the deformation in the manner of engineering elasticity. Not that it would be useless, but the just mentioned analysis of principal strains is more advantageous in the nonlinear range. The displacement vector and the infinitesimal strain tensor enter only at the stage of linearization. The shock waves and (coherent) phase fronts are sharp surfaces across which the deformation gradient and velocity have jump discontinuities (singular surfaces) but the actual position is continuous. The main consequence is the Hadamard lemma saying that the limiting values of the deformation gradient at the two sides of the interface are rank 1 connected. This opens the way to a number of essentially geometric topics, such as the mechanical theory of twinning, the austenite/martensite interface and others. The singular surfaces are assumed to bear no material structure: the surface tension, surface heating, and the surface concentration of mass are excluded. The transport theorems for processes with singular surfaces are proved. Then the balances of mass, momentum, energy, and entropy are introduced and their local forms for the bulk matter and for singular surfaces are derived.

Part II is somewhat independent of the rest. It deals with the foundations – the basic quantities of continuum thermodynamics, the total energy and entropy, are derived from a set of elementary axioms. For this, a state space formalism is introduced with a generality that covers also the memory phenomena and hysteresis. (This is also a basis for the general constitutive theory of materials.) There the reader will find statements of the first and the second laws of thermodynamics free from traditional ambiguities. The appealing programme of founding thermodynamics on the first and the second laws is achieved by simple but conceptually clear means. The theory resulting from Part II is the thermodynamics based on the Clausius–Duhem inequality, which is used throughout. There is no doubt about the appropriateness of this choice for the selected class of materials. Part II provides a strong support for this.

Part III describes the constitutive equations of viscous materials with heat conduction. The restrictions placed on the response functions by the Clausius–Duhem inequality, frame-indifference, and symmetry are derived. The only classes of symmetry to be dealt with explicitly are isotropic solids, fluids and crystals having the symmetry of the underlying Bravais lattice. Each of these classes has its own representation theorems. The approach to the representation theorems for isotropic solids is based here on the principal strains, principal stresses, and principal directions of strain rather than on the Rivlin–Ericksen representation theorem and the principal invariants. This sometimes provides a more direct way to fitting the experimental data on the empirical side and a somewhat better control over the convexity and ellipticity properties on the mathematical side. A discussion of the change-of-variables mechanism is given, emphasizing that each change of variables leads to a new quantity that can be useful for understanding certain aspects. Thus, for instance, Eshelby's energy momentum tensor is associated with the exchange of roles of the reference and actual configurations, besides being associated with the translational invariance in the reference configuration and phase transformations. In addition, a basis for the changes of the convexity properties under changes of variables is developed. Related to these are the thermodynamic coefficients – essentially the second derivatives of the thermodynamic potentials. These are the fourth-order tensors of elasticities (the elastic moduli), in isothermal and adiabatic versions, the coefficients of thermal expansion, the stress–temperature coefficients, the tensor of latent heats, and the scalar specific heats at constant deformation or stress. Some of these occur in the linearized equations in static and dynamic situations. The dynamic part of the response is treated similarly, which leads to the kinetic coefficients like the tensors of heat conductivity and viscosity etc. In addition, brief accounts are given of the classical linear irreversible thermodynamics and of its recent generalization–the extended irreversible thermodynamics.

Part IV is the theory of thermodynamic equilibrium. While Part II treats thermodynamics as the theory of heat and work, Part IV treats it as the theory of minima of integral functionals. The exposition starts with the thermodynamic background: in the conservative loading conditions, the canonical free energy decreases along processes. It follows that if an equilibrium state compatible with the external conditions is stable, the canonical free energy must take a minimum value among all states satisfying the kinematical constraints. The states that satisfy the extremum principles are examined assuming that they have the smoothness that allows a derivation of the Euler–Lagrange equations. This smoothness admits the singular surface; hence states of coexistent phases are included. The quasiconvexity along a minimizer is derived as a necessary condition for the minimum, as well as its consequence rank 1 convexity. Also the quasiconvexity at the boundary, equally important to the quasiconvexity itself, is shown to prevail on the free part of the boundary. While the quasiconvexity can be viewed as a condition for internal stability, the quasiconvexity at the boundary is a condition for the surface stability. It has been conjectured that its violation can cause surface wrinkling of certain metals.

The considerations are then applied to bodies of specified symmetry. For fluids this gives the classical thermostatics, treated in Part IV with the emphasis on the convexity/nonconvexity properties of the energy surface in the volume-entropy space. A rigorous proof of the Gibbs phase rule is given based on the Carathéodory theorem on the convex hull. The Gibbs function is shown to have singularities at the pressures and temperatures of phase transitions: Its supergradient must contain the specific volumes and entropies of all stable phases of the given pressure and temperature. Solids are treated first using the local approach, based on the linearization and implicit function theorem. This includes the linearized elasticity of stressed bodies and, as an extremely special but important case, the classical linear elasticity, i.e., the linearization about a stress-free state. For the general linearized elasticity, the positivity of the second variation is crucial for the existence and uniqueness of the solutions and for the absence/presence of bifurcations of the nonlinear equations. The general pointwise conditions on the tensor of elastic moduli related to the positivity of the second variation are discussed. These are the well-known strong ellipticity condition governing the behavior of the bulk matter, and the complementing and Agmon's conditions, controlling the surface phenomena. The latter appear to be less recognized explicitly, but the more enlightened portion of the elasticity literature treats the violation of the complementing condition under the name surface instabilities. The complementing and Agmon's conditions are discussed for isotropic states under tension or compression in some detail. A linear bifurcation analysis of a column under compression is presented as an example for the determination of parameters at which the uniform positivity of the second variation fails. Also an absence of instability under tension is explained for a model stored energy of the Blatz–Ko (special) type: at the tension, for which the principal forces are all nonnegative, the stored energy is convex. (In fact, one of this book's side goals is a rehabilitation of points of convexity, within limits. The folklore wrongly deems the convexity in the deformation gradient as 'contradicting the frame-indifference.')

The global theory of existence of solutions depends critically on the convexity properties of the stored energy and the related sequential lower semicontinuity of the total energy. The direct methods of the calculus of variations are the main working tools. For rubber-like materials the existence theory is based on a strengthened version of the quasiconvexity known as polyconvexity. The minimizers must be sought in the Sobolev spaces, and their quality depends dramatically on the exponent p in $W^{1,p}$. This is explained on the famous radial deformations with or without cavities. Also the devices to ensure reasonable versions of injectivity (invertibility) of deformations are reviewed in some detail. Unfortunately the book's size did not permit a systematic treatment, despite the author's opinion that a rather complete picture can be reconstructed from the existing literature. The polyconvexity, let alone rank 1 convexity, cannot be satisfied by crystalline bodies. In this case the total energy fails to be lower semicontinuous, and the properties of the minimizing sequences are not sufficiently fully reflected by the limiting macroscopic deformation. A finer device, Young's measure, must be used to encode the (spatial) oscillation phenomena occurring in the minimizing sequence. Physically, Young's measure describes the possible microstructures consistent with the given macroscopic deformation (in this context), and the set of all Young's measures may be viewed as an enlargement of the state space of the body.

Part V is about the dynamics. Besides the propagating phase boundaries mentioned above, this part deals with the dissipationless materials with shock waves, and with the resulting hyperbolic systems of equations. The current activities in the theory of hyperbolic systems involve one-dimensional models, susceptible to a fairly detailed analysis. Since the present book attempts to present general, three-dimensional bodies and the features common to responses of arbitrary symmetry, I found it necessary to present the entropy and Liu's criteria, Lax' inequalities, and the necessary background in this general setting. There appears to be no systematic treatment except for the isentropic case or fluids. The main problem is that the equations cannot be put in the form of a first-order system of conservation laws popular in fluid dynamics. Moreover, when the entropy is used as the independent thermal variable, which seems to be the only natural setting, the system does not have, even in the hyperbolic regime, a strictly (rank 1) convex mathematical entropy function: here the entropy is linear. The hyperbolicity, strict hyperbolicity, and genuine nonlinearity are formulated in this setting. The existence of the Hugoniot curve is proved locally, and the local equivalence of the entropy criterion with Lax' inequalities and Liu's criterion is established in the strictly hyperbolic, genuinely nonlinear regimes. The analogs of the centered waves of fluid dynamics are defined, and using this, the existence of the solution of the Riemann problem for nearly equilibrium initial data is proved through the implicit function theorem. Only then do I pass to fluids and show, using the classical analysis of Zemplén, Bethe, and Weyl, the global equivalence of the criteria for fluids satisfying the classical restrictions.

The presence of dissipation, e.g. the viscosity of the differential type, makes the problem of proving the existence of the time-evolution and examining its asymptotics easier. Despite that, the existing proofs deal only with one-dimensional models. Rather than these, this book includes only the proof of the existence of the time evolution of the model linearized at an equilibrium state of a solid. Even though the proof uses standard means, it is presented because in this case the ideal goal of the theory can be carried out to the end: the realistic conditions for the existence of evolution are given and the asymptotic properties, i.e., the trend to equilibrium, is proved when the second variation of the stored energy is positive definite. Moreover, efficient Liapunov functions can be calculated explicitly.