David R. Axelrad · Wolfgang Muschik (Eds.)

Constitutive Laws and Microstructure

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Proceedings of the Seminar
Wissenschaftskolleg – Institute for Advanced Study
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Foreword

The Wissenschaftskolleg zu Berlin, the first Institute for Advanced Study in Germany, was founded in 1981. According to its charter, the Kolleg's purpose is to promote scholarship by promoting scholars. To this end 40 outstanding researchers are invited each Academic Year by the Kolleg to develop, to continue or to complete a project of their choice. The Wissenschaftskolleg chooses its members without regard to country of origin, discipline or academic rang. During the year seminars devoted to themes deriving from Fellows' ongoing projects are organized.

This book is the result of such a seminar. Professor D.R. Axelrad who was a Fellow at the Kolleg in 1986/7 organized it in close cooperation with colleagues from the Technische Universität Berlin, notably Professor W. Muschik. For several reasons I am grateful to both editors and to the participants in the seminar.Their book demonstrates the opportunity given to members of the Wissenschaftskolleg to work on scientific syntheses, whether alone or in cooperation, which at the same time open new perspectives for research. <u>Constitutive Laws and Microstructure</u> is the result of a joint enterprise between the Kolleg and the universities and research institutions in Berlin.

Among the participants in the seminar were former, current and future fellows and friends of the Kolleg. I would like to thank all of them and Professors Axelrad and Muschik in particular for pointing out in such an impressive way the continuity of the work at the Wissenschaftskolleg.

Wolf Lepenies
Rektor, Wissenschaftskolleg zu Berlin

Preface

This book contains the invited papers of the Seminar on "Constitutive Laws and Microstructure" held at the Wissenschaftskolleg (Institute for Advanced Study) Berlin, West Germany, Febr. 23-24, 1987. The Seminar was held in cooperation with the Institute of Theoretical Physics and the Hermann Föttinger Institute of the Technical University, Berlin with the purpose of discussing some recent developments in the theory of materials. Unfortunately, due to the time-limit set for the Seminar and the restriction on the number of participants, it was not possible to cover a wider range of topics. However, an attempt was made to deal with fundamental issues of material theories and to indicate possible ways in which future research may aid in the formulation of more rigorous material theories.

The main topics of the Seminar include the thermodynamics of solids, constitutive relations on the basis of stochastic process theory, the molecular dynamics of simple fluids and the microphysics of polymers as well as the electro-magnetic control of properties in multipole materials.

The Seminar was sponsored by the Otto and Martha Fischbeck foundation and the Institute for Advanced Study, Berlin.

We would like to thank the rector of the Institute Prof. W. Lepenies for his support and hospitality that were extended to all participants. We would also like to thank the staff of the Institute for the perfect organization and their assistance during the Seminar.

Berlin, Montreal
Oct. 1987

D.R. Axelrad and W. Muschik

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Part I

Thermodynamics of Materials

Thermodynamical Constitutive Laws - Outlines -

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Summary

Material theories can be divided into two classes, the probabilistic and the deterministic or phenomenological theories. The probabilistic theories can be decomposed into stochastic, statistical and transporttheoretical branches which are shortly discussed. The phenomenological theories can be divided into two categories, those of discrete systems and those using continuum theoretical concepts which are discussed in more detail.

1. Introduction

The field of Constitutive Laws is wide and many-sided because the numerous different kinds of material properties can be described by different theoretical concepts. Especially in thermodynamics almost an inflation of distinct but related theories can be recognized so that constitutive laws taking into consideration also thermodynamical aspects can be synthesized in a great variety. Consequently this contribution introducing our seminar can only be a rough draft without achieving completeness presenting a selection of some representative methods and ideas concerning the theory of thermodynamical constitutive equations.

Material theories are divided into two classes, the *probabilistic* and the *deterministic theories* (Fig.1). The probabi-

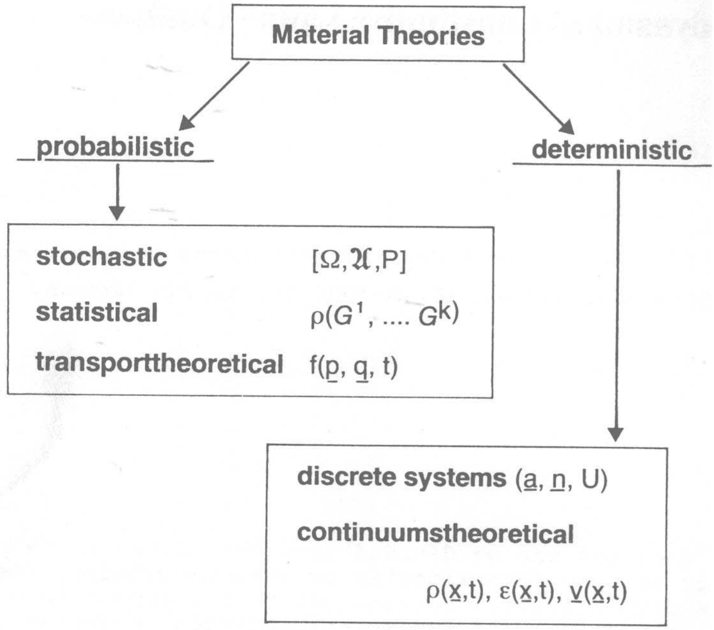

Fig. 1. Diagram showing distinct classes of material theories

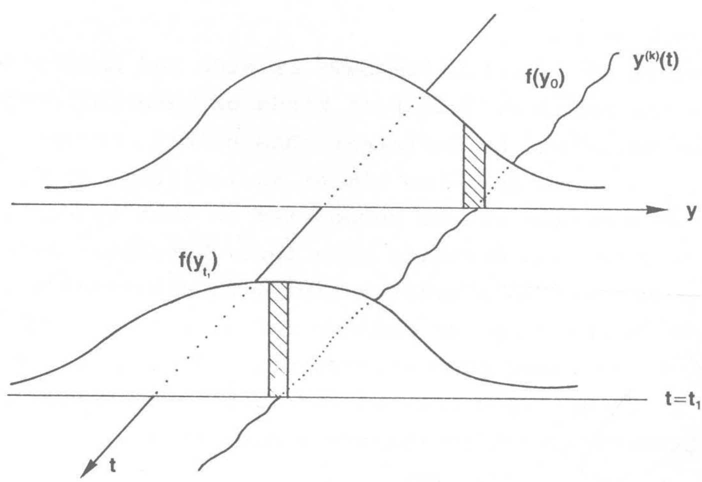

Fig. 2. Representation of a stochastic process by one of its realizations y^k (t) and its distribution function $f(y_{t_1})$ at time t_1.

tic theories themselves are decomposed into *stochastic*, *tistical*, and *transporttheoretical* branches which are rating with totally different probabilistic concepts. The ...ministic theories are split up into those which describe *crete systems* and others which deal with *continuumtheoreal concepts* being in principle different from those of ...ete systems [1].

Probabilistic Material Theories

rst of all I want to introduce the probabilistic material ieories and especially the stochastic ones because we are ll obliged to Professor Axelrad for this seminar, and he is ne of the promoters of stochastic mechanics of discrete media 2]. Stochastic constitutive theories are characterized by a easure space [Ω, A, P] - a Kolmogorov probability algebra - hich is interpreted in a special kind as we will learn below. Statistical theories are marked by a distribution function or by a density operator ρ which may depend on a relevant set of observables (so called Beobachtungsebene) [3] $G^1, \ldots, G^k$. Transporttheoretical methods also use a distribution function $f(\underline{p}, \underline{q}, t)$ which is defined in contrast to the distribution functions of the statistical methods on the (2f + 1)-dimensional μ-space of the single molecule having f degrees of freedom [4].

2.1 Stochastic Material Theories

The typical characteristic of stochastic constitutive theories is the division of the material into *microdomains* $^{\alpha}M$ and *mesodomains*

$$M^k = \bigcup_{\alpha \in I^k} {}^{\alpha}M \, . \tag{1}$$

Here the $I^k \subset N$ is a subset of the natural numbers counting the microdomains which the k-th mesodomain consists of.

The *state of the microdomain* $^{\alpha}\underline{s}$ is defined by a set of random variables which are elements of a random state space

$$^{\alpha}\underline{s} \in \Omega. \tag{2}$$

Subsets of this state space are called *events*

$$A \subset \Omega, \quad A \in \mathcal{A} \tag{3}$$

and are endowed with a *probability measure* P(A). Because all the introduced concepts refer to a microdomain $^{\alpha}M$ and to a special time t this microdomain and its state are described by a *Kolmogorov probability algebra* $[\Omega, \mathcal{A}, P]^{\alpha}_{t}$.

The constitutive equation of a microdomain $^{\alpha}M$ is expressed by the *local material operator*

$$^{\alpha}m: \quad ^{\alpha}\underline{s} \mapsto {}^{\alpha}\underline{Z} = {}^{\alpha}m({}^{\alpha}\underline{s}) \tag{4}$$

which maps the state of the microdomain onto its dependent material properties $^{\alpha}\underline{Z}$. The evolution in time is represented by an evolution operator

$$L_{t,t'} [\Omega, \mathcal{A}, P]^{\alpha}_{t'} = [\Omega, \mathcal{A}, P]^{\alpha}_{t} \tag{5}$$

which maps the probability algebra belonging to the time t' into that of time t. The evolution operator has the usual Chapman- Kolmogorov property

$$L_{t,t'} L_{t',t''} = L_{t,t''} \tag{6}$$

by which transition probabilities are defined

$$P^{\alpha}_{t} (A^{\alpha}_{t}) = \int dt' \, P^{\alpha}(A^{\alpha}_{t} \mid A^{\alpha}_{t'}) \, P(A^{\alpha}_{t'}), \tag{7}$$

$$A \subset \Omega^{\alpha}_{t}, \quad A^{\alpha}_{t} \in \mathcal{A}^{\alpha}_{t} \tag{8}$$

The *state* $\underline{s}^{k}$ *of the mesodomain* M^{k} is defined by the mean value of all microdomains which the mesodomain consists of:

$$\underline{s}^k(t) := \langle {}^\alpha\underline{s} \rangle^k(t) \equiv \sum_{\alpha \in I^k} {}^\alpha\underline{s}\, P(A_t^\alpha). \tag{9}$$

As the local material operator a *meso material operator*

$$m^k : \underline{s}^k(t) \longmapsto \underline{Z}^k(t) = m^k(\underline{s}^k(t)) \tag{10}$$

is defined which operates on and maps into random variables due to different realizations of the mesodomain by microdomains. By this meso material operator m^k a probability measure $P(\underline{Z}^k)$ is given on its range because on its domain another probability measure $P(\underline{s}^k)$ is defined by (9). Both material operators ${}^\alpha m$ and m^k are no measuring quantities because constitutive properties are measured in the macroscopic domain and neither on a microscopic nor on a mesocopipic level. Therefore we identify the mesodomain with the material coordinate

$$(\quad)^k \Longrightarrow \underline{X} \tag{11}$$

and by $P(\underline{s}^k)$ in relation with $P(\underline{Z}^k)$ we get the *stochastic material operator*

$$M_{\underline{X},t} : P(\underline{s}_t(\underline{X})) \longrightarrow P(\underline{Z}_t(\underline{X})). \tag{12}$$

This operator is defined on the probability measure of the stochastic process $\underline{s}_t(\underline{X})$ (fig. 2) and maps into the measure of the range of the constitutive equations $\underline{Z}_t(X)$ (fig. 3).

The stochastic material operator can be determined because the meso-state $\underline{s}_t(\underline{X})$ and its probability measure can be found out experimentally [5], and if the meso material operator is known or presupposed (12) becomes

$$P(m_{\underline{X}}(\underline{s}_t(\underline{X})) = M_{\underline{X},t}(P(\underline{s}_t(\underline{X}))). \tag{13}$$

Examples of this procedure have been given in several publi-

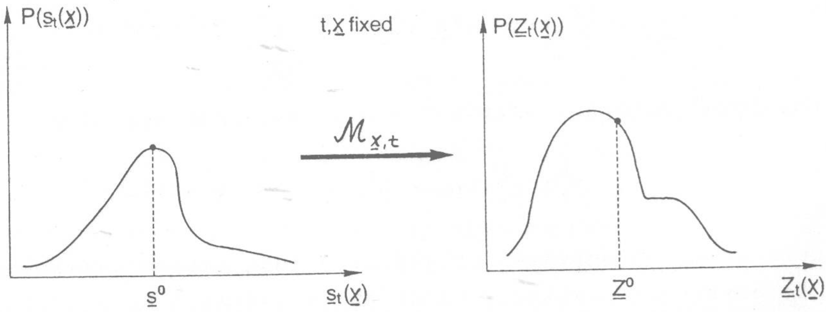

Fig. 3. The stochastic material operator maps the distribution function $P(\underline{s}_t(\underline{X}))$ of the state s at time t and position $\underline{X}$ into $P(\underline{Z}_t(\underline{X}))$ the distribution function of the material property $\underline{Z}_t(\underline{X})$.

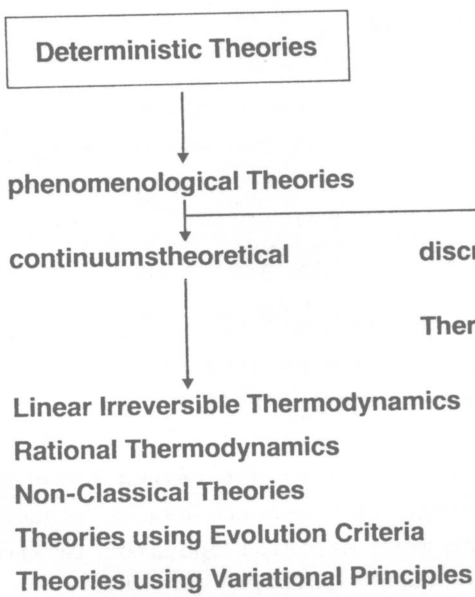

Fig. 4. Family of deterministic theories

cations [6].

2.2 Statistical Constitutive Theories

We consider a system which is described quantumstatistically: Its state by a *density operator* ρ with normalized trace for getting quantumtheoretical mean values $\langle F\rangle$

$$\mathrm{tr}\rho = 1, \quad \mathrm{tr}(F\rho) = \langle F\rangle, \tag{14}$$

its material properties by a *Hamiltonian*

$$H = H(p_1, \ldots, p_f, q_1, \ldots q_f, t) \tag{15}$$

which is in general time dependent. Here the p_i are the momentum operators and the q_j the position operators, when f is the number of degrees of freedom of this many-particle system.

Thermodynamically the system is described by the set of relevant observables [7]

$$\{G^1, \ldots, G^k\} \quad , \quad G^j = G^{j+}, \text{ for all } j \tag{16}$$

which are selfadjoint and called *Beobachtungsebene*. To each choice of a Beobachtungsebene we get a *generalized canonical operator* [8], [9]

$$R = Z^{-1} \exp(- \Sigma_j \lambda_j G^j), \tag{17}$$

$$Z = \mathrm{tr} \exp (- \Sigma_j \lambda_j G^j). \tag{18}$$

The c-numbers λ_j are determined by the k equations

$$\mathrm{tr}(G^j R) = \langle G^j\rangle = \mathrm{tr}(G^j \rho). \tag{19}$$

The *statistical entropy* is defined by

$$S := \mathrm{tr}(R \ln R) \geq \mathrm{tr}(\rho \ln \rho). \tag{20}$$