MATHEMATISCHES FORSCHUNGSINSTITUT OBERWOLFACH

Tagungsbericht 5/1992

Thermodynamische Materialtheorien

2.2. - 8.2. 1992

Die Tagung wurde von den Professoren Wolfgang Bürger (Karlsruhe) und Ingo Müller (Berlin) geleitet. Es gab 33 Teilnehmer und 32 Vorträge über folgende Aspekte thermodynamischer Materialtheorien:

a) Phasenübergänge
b) Elastizität und Inelastizität
c) Pseudoelastizität
d) Innere Freiheitsgrade und Hemmungen
e) Kinetische Gastheorie
f) Wellenausbreitung
g) Erweiterte Thermodynamik.

Behandelt wurden die mathematische Formulierung von Materialgleichungen sowie die Lösung von Rand- und Anfangswertaufgaben für die zugehörigen Feldgleichungen. Großen Raum nahm die Diskussion von Stabilitätsfragen ein, da viele der jetzt aktuellen Materialien sich durch instabile und metastabile innere Zustände auszeichnen. Diese stellen für die analytische und numerische Behandlung Neuland dar. Ein weiterer Schwerpunkt war die Erweiterte Thermodynamik mit ihren symmetrisch hyperbolischen Feldgleichungen. Diskutiert wurde in diesem Zusammenhang der Vergleich von Theorie und Experiment sowie der Vergleich der phänomenologischen Thermodynamik mit der kinetischen Theorie.

Großen Anklang fand ein Abendvortrag von Professor Wolfgang Bürger über die Mechanik und Thermodynamik von Spielzeugen mit vielen interessanten Experimenten.

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Vortragsauszüge

Abendvortrag

W. BÜRGER

Brain Teasing - Mechanical and Thermal Toys

In the now traditional after-dinner talk on Tuesday I demonstrated toys and everyday physical phenomena in about 25 entertaining experiments. Starting with the "cabinet-maker's masterpiece", building a "Leonardo's bridge", explaining, among other things, the little rope-climber, colliding cylinders, the egg cooker's paradox, the famous drinking duck, a thermal rubberband turbine, some spinning tops including the Sakai top and the tippie top, and let finally a cross-wing boomerang return in the lecture room to make clear that the simplest theory of its flight is not so bad. Interpolation appeared to be no valid principle when applied to elliptic yo-yos. Emphasis was laid not just on explaining the observations but rather on the intellectual play with the phenomena, in which the audience was included. The latter was occasionallly confronted with apparent paradoxa which became the starting point to rethink the models.

Sektion: Phasenübergänge

H. W. ALT

A Model for the Dynamics of Non-isothermal Phase Separation

We present a model which has been proposed in a paper with I. Pawlow (ISNM 95, 1-26 (1990). It is based on a free energy density

$$F(u,\theta) = f(u,\theta) + \frac{\kappa}{2}\,|\nabla u|^2 \,,$$

where u is a phase fraction or a concentration density and θ the

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Kelvin temperature. Here f represents the homogeneous part, whereas the second therm contains the surface energy of interfaces. We include the case that $\varkappa$ depends on u and θ, a situation which occurs in polymer mixtures. The model is based on the total energy

$$\int_{\Omega} \frac{F(u,\theta)}{\theta} dx \ .$$

The dynamical behaviour is described by the Cahn-Hilliard or the Cahn-Allen equation together with an energy balance equation. It is shown that the system satisfies a Clausius-Duhem inequality. We point out the connection to a model of Penrose and Fife (Physica D 43, 44-62 (1990)), which we interpret as a special case of our model.

H. ALTENBACH

Modellierung und Berechnung Thermomechanischer Vorgänge mit Phasenübergängen

Gekoppelte thermodynamische Prozesse sind gekennzeichnet durch sich beeinflussende Veränderungen der Temperatur, der Werkstoffstruktur, der Spannungen und der Verzerrungen. Ausgehend von den phänomenologischen Konzepten der Thermomechanik werden die materialunabhängigen Gleichungen, die materialspezifischen Gleichungen sowie eine verallgemeinerte Wärmeleitungsgleichung formuliert. Die dabei auftretenden Kopplungen mechanischer und thermischer Aussagen werden ausführlich diskutiert und bewertet. Das theoretische Konzept wurde im Rahmen des FE-Programmsystems "COSAR" des Instituts für Festkörpermechanik numerisch erprobt. Aufbauend auf existierenden Programmbausteinen wurde ein neuer Prozessor zum Programmklassenwechsel (Mechanikprozessor/Prozessor zur Temperaturfeldberechnung) entwickelt. Einfachste Testbeispiele, für die analytische oder numerische Vergleichlösungen vorlagen, haben die Anwendbarkeit des theoretischen Konzepts und der FE-Formulierung bestätigt. Dies wird am

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Beispiel von gekoppelten thermomechanischen Problemen mit Phasenübergang demonstriert.

Ko-Autoren: I. Altenbach, C. Münch.

F. FISCHER

Micromechanics of Materials: A Thermomechanical Consideration of the Transformation Condition for Martensite and its Application.

Different approaches can be followed to develop a transformation condition for martensitic transformation:

- a microregion concept considering the energy balance for a microregion (usually a part of a grain) before and after its transformation into a martensitic variant;
- the energy balance at a moving martensitic front, e.g. in the case of a growing variant;
- a microscopic concept introducing averaged variables and as an additional internal variable the volume fraction ξ of a martensite; further a assumption on the energy dissipation is included.

The models are derived and evaluated. It is shown that the microregion concept agrees with the experimentally observed order of selection of martensitic variants. A concept is presented how to derive a kinetic equation describing the evolution of ξ in dependence on the temperature and the load stress state. A comparison with experimental results is presented.

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M. NIEZDODKA

Diffusive Phase Transitions - Models with Constraints

Diffusive phase transitions give rise to strongly nonlinear systems of evolution equations (reducing to standard Cahn-Hilliard equation in the simplest case of an isothermal binary system). To provide physical feasibility of the phenomenological set-up, an extended form of the thermodynamic potential accounting for constraints on the state of the system may be needed. This contributes to the possibility of reducing the model to the generalized Cauchy problem

$$J^*(v'(t)) + \partial\varphi^t(v(t)) + p(v(t)) \ni 0, \qquad t>0$$

$$v(0) = v_o$$

in an appropriate functional setting, with maximal monotone component $\partial\varphi^t(\cdot)$ (in charge of homogeneous bulk driving mechanisms and constraints) and Lipschitz continuous part p(•) (in charge of the multi-phase system structure) singled out. Results on the existence and uniqueness of t-global solutions are reported together with an asymptotic analysis as t → ∞. Related questions discussed are on the system behaviour as the constraints become t-dependent, the possibility of treating the latter as a kind of control action that would contribute towards a prescribed terminal state structure and the dependence of the state of the system on perturbations of the thermodynamic potential.

Co-authors: N. Kenmochi and I. Pawlow

M. PITTERI

On the Variational Derivation of Equilibrium Equations for a Solid with a "Greasy" Phase Boundary.

I consider solids in which different phases coexist in equilibrium, also solids in equilibrium with their melts. I limit myself to mechanics, where I think the difficulties of the modelling are. In addition to bulk energy, I assume phase boundaries in solids, or between a solid and its melt, to have a certain surface energy function and compute its first variation. This provides surface forces to be added to bulk forces in the equilibrium equations for a body whith two phases co-exist in equilibrium. This problem has been considered by LEO & SEKERKA [1989]. I provide one variational frame for all the 3 types of interfaces they treat independently. In addition, I allow the body to be non-homogeneous, and consider body forces and dead loads on the boundary.

To develop the afore mentioned variational approach, I take advantage of results of GURTIN in his analysis of the mechanics of interfaces, in particular GURTIN [1989] and GURTIN, STRUTHERS & WILLIAMS [1989]. In this communication I restrict my attention to the case of two solid phases having an interface along which they can freely glide, while remaining in contact.

REFERENCES

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P.H. LEO & R.F. SEKERKA [1989], "The effect of surface stress on crystal- melt and crystal-crystal equilibrium", Acta Metallurgica 37, 3119-3130.

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I. SPREKELS

On the Fife-Penrose Model for Phase Transitions

The recent model of Fife and Penrose (Physica D, 1990) for phase transitions is considered. In terms of the order parameter e and the absolute temperature T, it leads to the initial-boundary value problem for the singular parabolic system

$$e_t - K\Delta e = -\frac{\partial F}{\partial e}(e,T) + a\,\frac{e}{T}\quad, \qquad (1)$$

$$T_t - aee_t + M\Delta\left(\frac{1}{T}\right) = g\quad, \qquad (2)$$

where K, M, a are positive constants, g represents the heat sources/sinks, and where F (●, T) (the free energy of the homomogeneous phases) is typically a double-well potential as function of e. For smooth data, it is shown that a unique global classical solution (e, T) exists, where T stays positive throughout. The main technical difficulty in the proof is to bound T positively from below. Numerical results representing the growth of a crystal with sixfold spatial symmetry from an undercooled liquid are presented.

Sektion: Elastizität und Inelastizität

M. HAYS

Shear, Shear Stress and Shearing

New formulae are derived for the shear of a pair of material elements within the contexts of infinitesimal strain and of finite strain. Also new formulae are derived for shear stress based on the (symmetric) Cauchy stress and for the rate of shear of a pair of material elements within the rate of strain theory.

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In particular a very simple short derivation is presented of the classical result of Coulomb and Hopkins on the maximum orthogonal shear stress.

Co-author: Ph. Boulanger

I. SHIH LIU

Interface Equilibrium and Inclusion Problems

The phenomenological description of solid interface in thermodynamic equilibrium has been widely investigated. Many of these treatments generalize Gibbs' classical result of phase equilibrium for fluid interface across which the chemical potential is continuous. Regarding the interface as a singular surface, from the usual jump conditions we derive the condition of interface equilibrium. This condition is more or less well established in the literature. For quasi-static processes, it is shown that Eshelby's energy-momentum tensor plays the role of the chemical potential in interface equilibrium.

We are interested in interfaces in a body conceived as a result of phase transition within a portion of the body, called the inclusion. Based on Eshelby's results for inclusions in a linear elastic medium, we examine the stability of the shape of the interface under infinitesimal transformation strains of dilatation and simple shear. It is found that an arbitrary inclusion subjected to a uniform dilatation can maintain its shape, while any inclusion bounded by a closed surface subjected to a simple shear can not.

A. MORRO

Thermodynamics of Visco-Elastic Solids

Thermodynamic restrictions on linear viscoelastic solids in the isothermal approximation are investigated by letting the work along approximate cycles be approximately non-negative (second approximate cycles). Necessary and sufficient conditions on the relaxation function are derived for the validity of the second law. The esential restriction turns out to be the negative definiteness of the half-range Fourier sine transform of the Boltzmann function. Definiteness rather than semidefiniteness is shown to be related to the concept of irreversibility which is given a precise definition. The role of the thermodynamic restrictions is examined in connection with some typical problems of wave propagation.

K. R. RAJAGOPAL

Inhomogeneous Deformations in Finite Elastic and Inelastic Solids

I shall first discuss the problem of determining a sufficiently large class of constitutive equations, within the context of compressible and imcompressible isotropic elastic materials, corresponding to a specific inhomogeneous deformation. Then, I shall consider specific inhomogeneous deformations, for special non-linear materials, which exhibit a "boundary layer" structure in that adjacent to the boundary the deformation is inhomogeneous and in a core region it is essentially homogeneous. Finally, I will also discuss a new theory for materials which undergo microstructural changes due to deformations. The prediction of such a theory within the context of some inhomogeneous deformations will be presented.

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Sektion: Pseudoelastizität

M. BROKATE

Numerical Simulation of Pseudoelastic Hysteresis Loops in Shape Memory Alloys

Müller and coworkers have proposed theoretically and validated experimentally a model to explain the stress-strain hysteretic relationship for shape memory alloys within the pseudoelastic range. Fedelich and Zanzotto have discussed a 1d nonisothermal extension of this model and have performed several numerical simulations. We present numerical simulations for the same problems, buth with a different numerical method based on an explicit treatment of the hysteresis operator and compare the results. There is a good quantitative agreement, but there are some qualitative differences related to the discontinuity of the model.

Co-author: J. Theel

Y. HUO

Thermodynamics of Pseudoelasticity

First the constitutive equation for shape memory alloy is propsed and investigated by using I^{st} and II^{nd} laws of thermodynamics. Then we try to study the energy dissipation mechanism in loading, heating processes. And we get the conclusion that two mechanisms are active and are responsible for the hysteresis phenomenon:

1. mechanical energy dissipated into heat
2. energy transported from higher temperature to lower one.

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I. MÜLLER

Thermostatics of Pseudoelasticity

Pseudoelasticity is a phenomenon that occurs in shape memory alloys. It is characterized by a hysteresis in the first quadrant of the load-deformation diagram. Loading leads to a phase transition from the austenitic to the martensitic phase and unloading reverses that transition. The thermodynamic treatment of the two-phase body in the transition makes use of a non-convex free energy and it supplements the usual terms with a coherency energy that is located at the internal interfaces. The minimization of the free energy leads to the conclusion that the hysteresis loop is diagonally crossed by a line of phase equilibrium. That equilibrium is stable for fixed deformation but unstable for fixed load. Therefore inside the hysteresis loop we may expect yield and recovery of deformation once the line of phase equilibrium is reached. Such phenomena are indeed observed and - by now - well documented. They are connected with significant changes in the number of interfaces which have not found a proper mathematical representation so far in the constitutive relations of pseudoelastic bodies.

K. TANAKA

Thermodynamic Models of Pseudoelastic Behavior of Shape Memory Alloys

Within the framework of classical thermodynamics two workable models of pseudoelastic behavior of shape memory alloys are developed. The so called R-model undergoes only reversible processes and constitutes the generalization of classical Maxwell model of phase transformation. The other model (R_L-model) includes interaction energy. It predicts formation of external and internal hysteresis loops, and complies with the Clausius-Duhem inequality.

The full set of coupled incremental constitutive relations are derived for both models. They enable us to determine phase compositions, stress and heat exchange with the surrounding under imposed strain and temperature variations, and are presumed to be valid at complex stress state. A specific form of the kinetic law for phase transformations is suggested which implies that at most 10 constants fully describe the pseudoelastic behaviour of isotropic alloys.

K. WILMANSKI

On the Metastability of States inside of the Pseudoelastic Hysteresis Loop

Recent experimental works have shown that the state of a single crystal, undergoing stress-induced martensitic transformation, is determined not only by the over-all deformation and the force (and, hence, by volume phase fraction and deformation) but also by an additional internal variable. In order to predict the path of the process inside of the force-deformation hysteresis loops, one needs at least three state variables such as (*force, deformation, number of interfaces*) or (*deformation, volume phase fraction, number of interfaces*). All these states are metastable, while the thermodynamic phase equilibrium - in contrast to, for instance, fluid-vapour phase transformations - is unstable, which is the consequence of the presence of coherence energy of interfaces.

The purpose of the present paper is to construct a model, explaining the metastability of such internal states of hysteresis loops in terms of appropriate semi-microscopic potentials, whose garland-like shape describes the local energy barriers for the progress of phase transition. These barriers stabilize the states outside of the unstable phase equilibrium line and, simultaneously, determine the triggering of one of the two mechanisms of phase transformation - either the growth (i.e. propagation of interfaces) or the nucleation (i.e. creation of new interfaces).

G. ZANZOTTO

One-Dimensional Quasistatic Non-Isothermal Evolution of Shape Memory Material inside the Hysteresis Loop

We study the quasistatic nonisothermal processes of a one-dimensional bar consisting of a two-phase shape-memory material. The system of p.d.e's governing the evolution of the bar is obtained by means of a temperature-dependent hysteretic stress-strain law that we formulate as a "plasticity" criterion and a hysteresis operator. The constitutive theory is developed here on the basis of the mixture approach proposed by Müller [1] and of a natural extrapolation of the isothermal experimental data regarding the behavior of the material inside the hysteresis loop recently described by Müller and Xu [2]. Numerical simulations are presented for three initial and boundary-value problems of interest with regard to uniaxial stretching experimental tests. See also the talk by Prof. M. Brokate at this same meeting.

[1] Müller, I.: "On the size of hysteresis in pseudo-elasticity", Cont. Mech. Thermodyn. 1 (1989), 125-142.

[2] Müller, I.: Xu, H.: "On the pseudo-elastic hysteresis" Acta Metall. 39 (1991) 263-271.

Co-author: B. Fédélich.

Sektion: Innere Freiheitsgrade und Hemmungen

G. BOILLAT

Involutive Constraints

M. FREMOND

Materials with Internal Constraints. Applications to Solid Mechanics and to Collisions

The state quantities of a material or of a structure can be submitted to internal constraints, for instance a volumetric proportion is positive, the distance of a point to a rigid body is positive, etc.

We decide to take these internal constraints into account with the free energy. We decide the value of the free energy to be $+\infty$ for non feasible states (for instance, for a negative proportion or an interpenetration of a point and a rigid body). We show that it is possible to overcome the difficulties due to the non smoothness of the free energy. The reactions to the internal constraints are in some sense the derivatives of the free energy. Examples are given: mixtures, phase changes, contact with adhesion damage, incompressibility, collision of a point and a rigid body.

K. HUTTER

Electrodynamics on a Surface

From the global statements in three dimensions a complete local theory of mechanical as well as electrodynamic field equations is derived in two dimensions for a curved phase boundary. The electrodynamic development is motivated by the classical point charge model and is restricted to non-relativistic phenomena. It turns out that the electric quadrupole moment is crucial. Without it, definition of electromagnetic surface fields is superfluous, as they vanish and the classical electromagnetic jump conditions emerge.

Co-author: A. Sadiki

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R. D. JAMES

Theory of Magnetostriction with Applications to $Tb_xDy_{1-x}Fe_2$

In this talk we discuss recent research on magnetism and magnetostriction with particular attention to the material $Tb_xDy_{1-x}Fe_2$, the material that exhibits the largest known magnetostriction. This material exhibits a complex and highly mobile domain structure consisting of both structural and magnetic domains. Typical growth habits for these crystal result in specimens with parallel twinned layers; these twinned layers remain fixed relative to the material during the magnetostrictive process.

We present a new theory of magnetostriction due to David Kinderlehrer and the author and discuss applications to the material $Tb_xDy_{1-x}Fe_2$. In the talk we explore in particular the role of the growth twins on magnetostriction. The currently held view among experimentalists is that these growth twins inhibit magnetostriction. We question that view and provide some evidence that they promote magnetostriction. The basic hypothesis here is that certain special kinds of composites of magnetostrictive materials may exhibit higher magnetostriction than single crystals by limiting the possible compatible domain structures. We also briefly discuss this possibility for martensitic materials.

F. M. LESLIE

Continuum Theory for Smectic Liquid Crystals

Initially this paper describes a new approach to the derivation of continuum theory for liquid crystals based solely on the balance laws for linear and angular momentum and the related concepts of force and moment, without appeal to generalized forces or torques. Constitutive relations follow from a rate of work assumption, namely that the rate of work by external forces and moments either goes into changes of kinetic and a Frank-

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Oseen energy, or into viscous dissipation, and as an illustration a resumé of nematic theory is given using this method.
In recent years, however, there has been considerable interest in deriving continuum models for smectic liquid crystals given their potential for applications in display devices. The remainder of the paper is therefore devoted to the description of a contimuum model for non-chiral smectic C liquid crystals, which adopts the two constraints, that the thickness of the layered structures on these anisotropic liquids remains constant, and also that variations in the tilt of the alignment with respect to the layer normal can be ignored. With these assumptions a constrained biaxial theory is derived by the method described above. Thereafter the paper attempts to assess progress achieved with this theory describing among other things static solutions for configurations involving parabolic cyclicles, and also solutions to some dynamic problems.

Sektion: Kinetische Gastheorie

C. CERCIGNANI

A Approach to the Chapman-Enskog Expansion

As is well-known, the Chapman-Enskog expansion is the bridge between the kinetic theory of gases and a macroscopic description of gas dynamics. Usual presentations are formally rather complicated, so that the formalism tends to obscure the significance of the method. In the talk, a suitable rearrangement of the Boltzmann equation is introduced, in such a way that the Chapman-Enskog expansion appears as the natural iterative solution when the Knudsen number (ratio of the men free path to a macroscopic length scale) is small. This approach also clearly exhibits the singular nature of the expansion and the necessity of introducing boundary layers where the expansion fails.

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G. M. KREMER

A Generalization of the Method of Grad

By using the method of Chapman-Enskog as a base, we have determined successive approximations of any order to the transport coefficients of shear viscosity and thermal conductivity for a monatomic ideal gas. The expressions for the transport coefficients involve only integrals which can be evaluated once the law of interaction between the spherically symmetric particles is known. Moreover, we have developed a (13 + 9N)-field theory based on the method of Grad and showed that the transition from this theory to a five-field theory leads to the same results as those obtained by the method of Champan-Enskog.

J. SCHRÖTER

Correlational Thermodynamics and the Problem of Transport Equation in Plasmas

The starting point is a kinetic theory for pair distribution functions describing plasmas. The interaction between the charged particles of the plasmas is the complete electromagnetic interaction with a finite speed of propagation. Forming moments, from this theory the balance equations of correlational thermodynamics are derived. Using Grad's method, as an example correlational thermodynamics of first order is considered. The resulting integro-differential equations are solved approximately. The result is used to calculate the conductivity of plasmas.

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K. SUCHY

Evolution Equations for Orthogonalized Moments in Mixtures of Gases

For gas mixtures without internal degrees of freedom the Boltzmann equations for the different species are coupled by the collision integrals. For transport processes near local thermodynamic equilibrium the velocity distribution functions are expanded using three-dimensional orthogonal Hermite polynomials with the local Maxwellians as weight functions. The latter are centralized with the mean mass velocity of the whole gas and normalized with an overall temperature. For the expansion coefficients a coupled system of evolution equations is established. The coefficients of the polynomials of first and third order are proportional to the diffusion flux vectors and the heat flux vectors, respectively. The approximated equations for these flux vectors form a linear inhomogeneous system with a singular symmetric matrix of coefficient. The vanishing sum of the diffusion flux vectors makes these vectors linearly dependent. This property is used to solve the linear system with a symmetric solution matrix. Summing the heat flux vectors to the total heat flux vector this symmetry leads to the Onsager symmetry relation.

Sektion: Wellenausbreitung

K. KIRCHGÄSSNER

On the Non-linear Dynamics of Travelling Fronts

Nonlinear waves in conservative - or dissipative systems generate their own dynamics. A gauge transformation is presented which brings the original equation into a form containing the given wave as an isolated steady solution. The space in which to define the dynamics follows then in a natural way. For the case of the Kolmogorov equation the long time asymptotics of perturbations is determined and extensions to systems and to the PDE's of water waves is indicated.

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H. ZORSKI

Heat Waves in One-Dimensional Fluids - The Parabolic Case

We construct particular solution-waves propagating with a finite speed, for non-hyperbolic systems (degenerate parabolic in the case of the heat conduction equation), describing some one-dimensional fluids and solids. The considered self-similar solutions depend on one variable $\zeta = x - c\,t$ only and the existence of the considered waves is connected with the existence and nature of the fixed points of a system of ordinary differential equations. The two regions (the perturbed and the unperturbed one) can be regarded as two phases and the construction of the particular solutions establishes collisions under which the two phases can coexist. Our problems resembles the search for solutions in particular systems of partial differential equations.

Sektion Erweiterte Thermodynamik

W. DREYER

A Test on Thermodynamic Theories: The Heat Pulse Experiment

A heat pulse experiment has been made with various crystals at very low temperature (1°K - 20°K). As an idealisation we have considered the crystal as an one-dimensional heat conductor, which ranges from $x = 0$ to $x = L$, where L denotes its length.
At $x = 0$ a heat pulse was supplied to the crystal and at $x = L$ the temperature as a function of time t was measured.
The experiment has uncovered three energy transport mechanism and thus has led to a complex picture.
At very low temperature a heat pulse can traverse the crystal without changing its pattern. This pulse is called "ballistic pulse". If the temperature is raised, the original pulse is split into two pulses. The first one suffers a strong damping and disappears after some time while the second pulse needs some

time for its development. This pulse is called "second sound". If we raise the temperature further the second sound pulse does not appear anymore and the ballistic pulse is followed by a long diffusive tail.

For the determination of the temperature we developed a system of field equations which rely on the phonon model and the phonon Boltzmann equation.

The mathematical structure can briefly be described as follows. N volume densities u_A ($A = 1,2,...N$) are considered to be the thermodynamic variables for which an initial-boundary-value problem has to be solved. The field equations are quasi linear PDE's of symmetric hyperbolic type with a convex extension.

We considered and solved several initial-boundary-value problems and could show that there is complete agreement with the experimental data for the three regimes described above.

W. LARECKI

Hyperbolic Equations of Transport and Thermal Waves Derived from an Approximate Thermal Description of Phonon Processes

Phonon gas hydrodynamics based on balances of energy and quasi-momentum and involving phonon distribution function which maximizes the entropy is considered for the case of a single branch of phonon excitations. The resulting field equations assume the form of symmetric conservative system with respect to the fields of the Langrange multipliers of the variational problem of entropy maximization. For the linear isotropic approximation of the phonon frequency spectrum and the phonon wave-vector domain approximated by the whole space, this system is explicitly determined and its global hyperbolicity is proved. Obtained equations of phonon gas hydrodynamics are rearranged to the form of conservation equations for energy and heat flux which can be considered as the extended thermodynamics of a rigid heat conductor. For this system, the propagation of thermal waves of weak discontinuity is analyzed.

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T. RUGGERI

Mathematical Problems in Extended Thermodynamics

The aim of modern Extended Thermodynamics is to deduce (using a rational procedure) the set of hyperbolic equations governing thermodynamical processes for a non-equilibrium gas. The limitation is that the theory is valid only for processes that are not far from equilibrium. The first problem that we discuss is the determination of the maximal distance from the equilibrium state for which the theory is consistent with the axioms. As a second problem we discuss thermo-acceleration waves and shock formation. Finally we present some differences between the classical and the relativistic case with respect to the problem of convexity, symmetrization and well-posedness.

W. WEISS

Determination of Transport Coefficients in Equilibrium

The transport-coefficients shear-viscosity, bulk-viscosity and heat-conductivity, which appear in thermodynamics, can be determined in several ways. One method relies on the fact, that a body which is in macroscopic equilibrium on a more microscopic scale shows non-equilibrium fluctuations, that never come to rest.

The information that is contained in the fluctuations can be used to determine the transport coefficients. By using the Onsager hypothesis, which relates the fluctuations to the thermodynamic fields, one can derive the so called Kubo-formulae, which are to be found in textbooks on statistical mechanics.

In this lecture the modified Kubo-formulae were evaluated by several methods. We used

i) BBGKY-Hierarchy

ii) Extended-Thermodynamics,

iii) Molecular-Dynamics.

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Concerning the shear viscosity and the heat conductivity all methods agree fairly well. The Kubo-formula for the bulk-viscosity, however, lead to the result that Extended Thermodynamics and Molecular Dynamics agree fairly well, while there is a complete disagreement between the bulk-viscosity coming from these methods and the one that is derived in the framework of the BBGKY-hierarchy.

Berichterstatter: I. Müller

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