Mathematisches Forschungsinstitut Oberwolfach

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Thermodynamische Materialtheorien

December 15th – December 21st, 2002

The meeting was organized by Kolumban Hutter (Darmstadt), Ingo Müller (Berlin) and Lev Truskinovsky (Minneapolis). There were 46 participants, of which 33 presented talks during the morning and afternoon sessions.

The meeting was focused on researches in the broad field of thermodynamic material theories. The talks were conducted on main topics involving

- extended thermodynamics,
- phase transitions,
- nonlinear elasticity,
- plasticity,
- micro- and macromechanics of crystals,
- relativistic mechanics,
- stability, homogenization, existence of solutions.

An after-dinner talk on Granular Materials was presented by K. Hutter. It was a lecture – exposed by means of photographs and laboratory experiments – on unsolved problems in avalanches of snow and debris, affecting human life and our environment.

Friday morning was devoted mostly to the presentation of some open problems in thermodynamics of materials.

The coffee and lunch breaks and, not at last, the random disposal of the participants around the tables in the dining-room, encouraged fruitful individual discussions. Many thanks are addressed to the MFO staff for the pleasant atmosphere and excellent working conditions.

The meeting turned out to be an illustrative example of cooperative research involving the fields of mechanics and pure mathematics. The abstracts of the talks are given below in alphabetical order.

Abstracts

Justification of homogenized models for viscoplastic bodies with microstructure

HANS-DIETER ALBER (DARMSTADT)

We discuss the homogenization of the quasi-static initial-boundary value problem with internal variables, called the microscopic problem, which models the behaviour of viscoplastic bodies at small deformations. This problem consists of the equations

$$-\mathrm{div}_x\, T_\eta(x,t) = b(x,t)\,,$$

$$T_\eta(x,t) = D(\frac{x}{\eta})\big(\epsilon(\nabla_x u_\eta(x,t)) - Bz_\eta(x,t)\big)\,,$$

$$z_{\eta\,t}(x,t) \in g\big(\frac{x}{\eta}\,,\, B^T\, T_\eta(x,t) - Lz_\eta(x,t)\big)\,,$$

$$z_\eta(x,0) = z_0^{(0)}(x,\frac{x}{\eta})\,,$$

$$u_\eta(x,t) = \gamma(x,t)\,,\quad (x,t) \in \partial\Omega \times [0,\infty)\,.$$

Here $u_\eta(x,t) \in \mathbb{R}^3$ is the displacement of the material point $x \in \Omega$ at time t, $T_\eta(x,t)$ is the Cauchy stress tensor, and $z_\eta(x,t) \in \mathbb{R}^N$ is the vector of internal variables. It is assumed that the elasticity tensor $D[\,y]$ and the "constitutive function" $z \to g(y,z)$ depend periodically on the variable $y \in \mathbb{R}^3$, which implies that the body modelled by the equations above has a periodic microstructure with the scaling parameter $\eta > 0$. Also, $z \to Bz = \varepsilon_p$ is a linear mapping, which assigns the plastic strain tensor ε_p to the vector z of internal variables, and L is a positive semi-definite $N \times N$–matrix.

We show that under suitable assumptions stated below the homogenized system formally derived from this initial-boundary value problem is justified: To this end it is first shown that the homogenized system has a solution (u_0, u_1, T_0, z_0). With this solution the asymptotic series

$$\hat{u}_\eta(x,t) = u_0(x,t) + \eta\, u_1(x,\frac{x}{\eta}\,,t)\,,$$

$$\hat{T}_\eta(x,t) = T_0(x,\frac{x}{\eta},t)\,,$$

$$\hat{z}_\eta(x,t) = z_0(x,\frac{x}{\eta},t)$$

is formed, and it is shown that the difference of the exact solution (u_η, T_η, z_η) and the asymptotic solution tends to zero if the scaling parameter η tends to zero.

Our results are proved for viscoplastic material behaviour that can be modelled by constitutive equations of monotone type with linear hardening terms. Moreover, we are only able to prove the convergence result locally in time and for smooth data. The reason for this last strong restriction lies in a technical problem: At one place in the proof the "energy method" of Tartar is used. The regularity properties for the asymptotic series solution required by this method are not satisfied by the global solution (u_0, u_1, T_0, z_0) of the homogenized problem; this restricts the result to local smooth solutions.

We surmise however, that the result can be extended to global solutions, possibly with a weaker convergence estimate.

On the structure of equations of macrophysics

VICTOR BERDICHEVSKY (DETROIT)

It was firmly established that equations of macro-physics must obey to the first and the second laws of thermodynamics. Are there other constraints? First such additional constraint for linear equations was found by Onsager. It follows from reversibility of micro-motion. This talk aims to show that there is much more rich structure of macro-equations which follows from Hamiltonian structure of micro-equations and holds for both linear and nonlinear cases.

A relativistic derivation of some nonlinear limited flux diffusion equations

YANN BRENIER (NICE)

Nonlinear limited flux diffusion equations are well-known in the field of radiation hydrodynamics. They are supposed to describe interaction of photons and matter. A typical example is

$$\partial_t \varphi = \nu \nabla \cdot \frac{\varphi \nabla \varphi}{\sqrt{\varphi^2 + \frac{\nu |\nabla \varphi|^2}{c^2}}}, \tag{1}$$

where c is the speed of light and ν is a diffusion coefficient. This equation has a finite speed of propagation c. In my talk I show how (1) can be derived from the scheme designed by Kinderlehrer-Jordan and Otto (SIAM Math. Anal. 29, 1998), provided the "kinetic energy distance" (the so called Wanerstein distance) is replaced by its relativistic counterpart.

Pattern formation in rate-independent plasticity

PAOLO CERMELLI (TORINO)

I have presented a model for the formation of dislocation cells and walls in the framework of rate-independent plasticity. The dislocation densities are introduced as primitive quantities related to the crystallographic structure of the material. These satisfy evolution equations which reduce to quasilinear parabolic PDEs with mobility proportional to the slip velocities. The model generalizes Kock's law for hardening to situations in which the dislocation densities are not uniform. Numerical simulations are also presented, which show the formation of cells in double slip.

Reconstructive phase transformations

SERGIO CONTI (LEIPZIG)

We study reconstructive phase transformations in crystals, in which the parent and the product lattices have arithmetic symmetry groups admitting no finite supergroup, the best known example of which is fcc-to-bcc in iron. We describe maximal Ericksen-Pitteri neighbourhoods, which characterize weak transformations. Focussing for simplicity to a 2D setting, we show how to construct a class of strain-energy functions which have the full $GL(2, Z)$ invariance, and are suitable e.g. for the study of the square-to-triangular reconstructive transition. Numerical simulations based on this energy illustrate the relation between reconstructive transitions, dislocations and plasticity in crystals.

On the Becker Döring theory of nucleation

WOLFGANG DREYER (BERLIN)

The Becker Döring (BD) model describes the evolution of droplets by two simple processes: A droplet with α atoms grows or shrinks by adding or subtracting a single atom, respectively.

Originally the BD model was designed to describe the evolution of liquid droplets which are in contact with a gas. Today it has become very popular to apply the model to the evolution of precipitates in solids. Our motivation to restudy the BD model results from the objective to simulate an elaborate process in single crystal gallium arsenide, where diffusion might lead to the formation of liquid arsenic droplets.

The underlying physics is embodied in the two transition rates for growth and evaporation appearing in the BD model and we determine these as follows: At first we start with the simple example of a single droplet in contact with its vapour. We argue thermodynamically as well as kinetically to calculate the transition rates. Next we transform these transition rates into an alternative but equivalent form, so that only terms appear which do not refer to the ideal gas example anymore. In the third step, the resulting transition is generalized to the case of a liquid droplet in contact with solid matter.

There are two reasons why the transition rates from a single droplet model can not simply be transferred to the many droplets model by summing up single droplet contributions. 1.)The free energy of mixing must be introduced additively, so that spontaneous nucleation which is not included in the single droplet becomes possible. 2.) The ratio of the rates is uniquely determined by the second law of thermodynamics, and this ratio is different in the single and in the many droplets model.

Fluid Mechanics with internal inertia

SERGEY GAVRILYUK (MARSEILLE)

We study a class of dispersive Lagrangian models including, in particular, bubbly fluid and shallow water models. We prove the analogs of well-known theorems of Fluid Mechanics for such models (Cauchy, Lagrange, Kelvin, etc.) and present some new particular solutions.

Effect of interfacial energy on binary phase diagrams

YONGZHONG HUO (SHANGHAI)

Interfacial energies affect the equilibrium in a binary solution or a binary alloy in which two phases coexist, e.g. liquid and vapour or solid and liquid. The criterion for equilibrium is provided by a minimum of the available free energy. The free energy is a function of

* the densities of the constituents
* the mol fractions in the phases
* the number of interfaces, and
* the phase fraction.

Under simplifying assumptions, i.e. when interfacial energies are ignored, the minimum of availability is determined by the common tangent rule for the Gibbs free enthalpies of the two phases. When the common tangent is projected into a (pressure, mol fraction)-diagram, a phase diagram results which - in the simplest case - is characterized by a single

two phase region. In a more complex case, characterized by the occurrence of a heat of mixing in the liquid phase, the well-known eutectic diagram occurs which exhibits a miscibility gap in the liquid and a triple point, the so-called eutectic point.

Once interfacial energies are taken into account, the two-phase regions become smaller and the eutectic point extends into a line element.

Moreover, the interfacial energies are the cause of nucleation barriers and the new phenomenon of the creation of kernels occurs, i.e. smallest entities of the new phase precipitating in a hitherto single-phase body.

Avalanching flows of snow, debris and mud – geophysical systems between order and disorder of matter

KOLUMBAN HUTTER (DARMSTADT)

Avalanches of snow, debris and mud are dynamical systems that, depending upon the conditions of loading may behave as solids or fluids or gases. This provides the basis for a rich behaviour between order and chaos. We begin by describing the distinguished features of granular materials such as dilatancy, solid, fluid and gase-like behaviour. We point out the role of the interstitial fluid if it is present, discuss Coulomb friction inside the material as well as at the boundaries and address liquefaction or fluidisation and particle size separation. All this will be illustrated, partly with photographs from natural events and partly with table experiments and videos. These typical features point at forms of descriptive models which will briefly be discussed.The talk ends with a number of experiments on flow-avalanches and shock formation in such flows.

Maximum entropy and consistent order ET

MICHAEL JUNK (KAISERSLAUTERN)

The consistent order moment system introduced by Müller, Reitebuch and Weiss is investigated and several structural features are presented: under suitable assumptions on the chosen polynomial weight functions, which define the moment variables of the system, Galilean invariance is recovered. Moreover, if the polynomial weights are scaling invariant, the system can be transformed into divergence form which is necessary to obtain a weak formulation. A further property is the consistency of the closure with the assumption of an exponential phase density. This density is obtained by solving a suitably defined maximum entropy moment problem, but since the set of moment constraints is non-convex, the maximum entropy approach fails to provide a nice entropy structure for the moment systems.

Constitutive modelling of ferroelectric ceramics

MARC KAMLAH (KARLSRUHE)

The piezoelectric effect is exploited by the poled state of ferroelectric ceramics. In the recent decade, there has been an increasing need to model their nonlinear, electromechanically coupled constitutive behaviour.

To begin with, the basic microscopic mechanisms found in the material and the hysteresis phenomena resulting on the macroscopic scale are discussed. Then, a general framework for constitutive models for ferroelectric ceramics is sketched, accounting for the recent

discussion in literature. A specific model formulation with respect to the choice of microscopically motivated internal variables representing the state of the microstructure is motivated. The basic model properties are discussed.

Molecular dynamic simulations of austenite $\leftrightarrow$ martensite transitions in 2D – phase stability and the principle of entropic stabilization

OLIVER KASTNER (BERLIN)

A 2-dimensional molecular-dynamic model for the investigation of crystalline phase transitions is presented. The model is based on the equations of motion, and Lenard Jones potential functions are employed.

Two types of atoms may create a stable square lattice, which is called the austenitic phase. It may transform into sheared variants, which represent martensitic phases.

In numerical experiments – examples are presented on a display screen during the talk – it is shown that the stability of the austenitic phase depends on temperature. Once stability is lost, the resultant phase transition exhibits strong similarities to martensitic transformations as they are known from shape memory alloys.

The temperature dependence of phase stability may be explained by the principle of entropic stabilization: Martensite is energetically more favourable, since it provides minimal internal energy U. Austenite, however, is entropically more favourable, since it provides maximal entropy S. The competition of both quantities is reflected in the free energy $F = U - TS$, which has to be minimal in phase equilibrium. Temperature T plays the role of a weight factor, which determines the influence of entropy.

The thermodynamic material properties of a small test body are numerically measured in tensile experiments. The free energy of the body is then determined from these data. Consequently the thermodynamic criterion of phase stability may be investigated.

Aspects of mechanics in material space

REINHOLD KIENZLER (BREMEN)
(joint work with G. Herrmann (Davos))

Remarkable hidden interrelations can be shown to exist between some fundamental principles of continuum mechanics if a four-dimensional formalism is used, e. g., if time is placed on the same footing as space. To exhibit these properties, the special theory of relativity supplies the proper framework. The fully relativistic energy-momentum tensor and the associated Euler-Lagrange equations are formulated for an elastic solid and for a perfect fluid as a limiting case. Approximate relativistic balance and conservation laws are then derived by expanding the exact relativistic relations in series of powers of the ratio of the velocity of motion to the velocity of light. Several orders of approximation are examined in detail, employing both the Eulerian and the Lagrangian description. This permits to gain new insight into the interrelated structure of the basic laws of continuum mechanics, such as the balance (or conservation) of mass, energy, physical (linear) momentum and material (linear) momentum. As a by-product, a hierarchy of approximate theories of continua is established whose velocity of motion is comparable to the velocity of light.

Keywords: continuum mechanics, special theory of relativity, balance and conservation laws.

Aspects of spatial evolution in some equations of continuum physics

ROBIN JOHN KNOPS (EDINBURGH)

The equilibrium equations for a nonlinear elastic cylinder exhibit a quasi-hamiltonian structure when the axial variable is regarded as a surrogate for time. It follows that behaviour in succesive cross-sections corresponds to evolution with respect to "time", while data specified on the base correspond to initial data. (The Cauchy problem is non-standard and indeed is ill posed since the equations remain elliptic.) Moreover, the "dynamical" structure suggests a relationship with Liapunov stability theory enabling various energy fluxes over plane cross-sections to be interpreted as "Liapunov" functions, although the derivatives and not the functions themselves now are non-negative. "Asymptotic instability" and "asymptotic stability" are equivalent to growth and decay with respect to large values of the axial variable. Such alternative "spatial evolution" accords with the classical Phragmen-Lindelöf principle of potential theory, and, in particular, the decay component relates to Saint-Venant's principle, important in studies of boundary layers and similar edge effects.

These ideas were applied to elliptic equations by Payne and Weinberger (1959) and were later further developed by several other authors especially in the context of elasticity. It is these later developments that are described here, largely for a linear anisotropic nonhomogeneous elastic cylinder. Only fixed lateral boundary conditions are considered either for ease of presentation or because the corresponding problems with a free lateral surface still await resolution. Of course, several other techniques have been employed in the investigation of Saint-Venant's principle and similar effects. One, however, that is closely allied to that under present discussion uses bulk (volume) energy measures and originated with Toupin (1965) and Knowles (1966). Nevertheless, the method based upon surface measures is preferred as it more transparently reflects the quasi-hamiltonian structure and does not obscure alternative behaviour.

The essence of the technique is a first order differential inequality for the surface energy flux. Integration generates estimates for alternative growth and decay in the form of exponentially increasing and decreasing lower and upper bounds respectively. The growth and decay rates depend explicitly upon the material parameters and the cross-sectional geometry, whereas the amplitude in the estimates additionally depends implicitly upon the base data. A subsidiary calculation is required to obtain an explicit dependence. Estimates may also be obtained for the decay of the mean-square displacement, strain, stress and displacement gradient. Extensions of the method to incompressible elasticity and non-steady Stokes flow are sketched and introduce the new feature of requiring two or more "Liapunov" functions.

It is shown how the same general approach may be applied to non-cylindrical regions including those with non-compact boundary, and with the plane surfaces for the energy flux replaced by level of parallel surfaces. This leads to the consideration of transverse decay in the elastic cylinder. The same approach also may be adapted to establish continuous dependence of the decay behaviour on the elasticities and on the base geometry for a cylinder. Briefly discussed is a selection of other problems in related fields of continuum physics that are amenable to the analysis, including some from linear elastodynamics.

Irreversible processes in cosmological models

GILBERTO M. KREMER (CURITIBA)

By using the thermodynamic theory of irreversible processes and Einstein general relativity, a cosmological model is proposed where the early Universe is considered as a mixture of a scalar field (inflaton) with a matter field (particles). The particle production process is represented by a non-equilibrium pressure in the energy-momentum tensor. The dynamic equations of the inflaton and the Einstein field equations determine the time evolution of the cosmic scale factor, the Hubble parameter, the acceleration and of the energy densities of the inflaton and matter. It is shown that in some regimes the acceleration is positive which simulates an inflation. The acceleration decreases and tends to zero in the instant of time where the energy density of the matter attains its maximum value.

We consider the present Universe as a mixture of a scalar field (dark energy) with a matter field (cold dark matter and baryons). The irreversible processes are also represented by a non-equilibrium pressure term in the energy-momentum tensor. In this case it is shown that a present acceleration with a past deceleration is a possible solution of the Friedmann equation. The dark energy density decays more slowly with respect to the time than the matter energy density does. The inclusion of the non-equilibrium pressure leads to a less pronounced decay of the matter field with a shorter period of past deceleration.

Fracture mechanical and micromechanical modelling of thermo-electro-mechanical materials

MEINHARD KUNA (FREIBERG)

The widespread application of piezoelectric and pyroelectric materials used as sensors or actuators in mechatronic, microelectronic and smart structures requires high strength and reliability under electrical, mechanical and thermal loads.

An introduction is given into the basic coupled anisotropic thermal, electrostatic and elastic constitutive equations for these materials. The singular behaviour of the coupled thermo-electro-mechanical fields at crack tips is discussed. Fracture mechanics concepts for the assessment of cracks in the above mentioned structures are presented. Finite-element-methods are reported to compute the coupled field problem and to determine the fracture controlling parameters.

Furthermore, a micromechanical model is presented for the fracture process zone in ferroelectric/ferroelastic materials, taking into account the non-linear domain switching phenomena. It explains the influence of the electric field on the fracture toughness of these materials.

Nucleation of dislocations and Kosterlitz-Thouless transition

KHANH CHAU LE (BOCHUM)

Thermal nucleation of screw dislocations in 2-D case is studied. We present the probability of N dislocation pairs to appear as a limit value of some functional integral and find an approximate value of this limit. The probability distribution of dislocation positions is studied within the same approximation. For small dislocation concentration the transition is of Kosterlitz-Thouless type, while at larger dislocation concentration the transition corresponds to nucleation of dipoles which remain bounded.

Energetic formulations for inelastic material behaviour

ALEXANDER MIELKE (STUTTGART)

The theory of standard generalized materials is based on two constitutive functions, namely the stored–energy density $\psi = \psi(x, F, z)$ and the dissipation potential $\Delta = \Delta(x, z, \dot{z})$. Here $F = \mathrm{D}\phi$ is the deformation gradient and z denotes the internal variables. The equations take the form

$$\begin{aligned} -\mathrm{div}\Big[\partial_F \psi(\mathrm{D}\phi, z)\Big] &= \ell(t,\cdot) \quad \text{in } \Omega, \qquad \text{bound. cond. on } \partial\Omega, \\ \partial_{\dot{z}} \Delta(z, \dot{z}) &= -\partial_z \psi(\mathrm{D}\phi, z) \quad \text{in } \Omega, \end{aligned}$$

where the first line is the elastic equilibrium condition and the second line is the balance for the internal conjugate forces (which is equivalent to the flow rule). For rate independent material laws we introduce the dissipation distance $D = D(z_0, z_1)$ on the manifold Z of internal variables via

$$D(z_0, z_1) = \inf\{ \textstyle\int_0^1 \Delta(z(s), \dot{z}(s))\,\mathrm{d}s \mid z(0) = z_0,\ z(1) = z_1 \}.$$

For $\phi : \Omega \to \mathbb{R}^d$, $z, \tilde{z} : \Omega \to Z$ we set

$$\mathcal{E}(t, \phi, z) = \textstyle\int_\Omega \psi(\mathrm{D}\phi(x), z(x))\,\mathrm{d}x - \langle \ell(t), \phi \rangle, \quad \mathcal{D}(z, \tilde{z}) = \int_\Omega D(z(x), \tilde{z}(x))\mathrm{d}x.$$

We replace the above system by the weaker energetic formulation given via

stability (S) and **energy inequality (E)**.

A pair of functions $(\phi, z)[0,T]\times\Omega \to \mathbb{R}\times Z$ is called solution of the **energetic formulation**, if for all $0 \le s < t \le T$ we have:

(S) $\mathcal{E}(t, \phi(t), z(t)) \le \mathcal{E}(t, \widetilde{\phi}, \widetilde{z}) + \mathcal{D}(z(t), \widetilde{z})$ for all $\widetilde{\phi}$ and $\widetilde{z}$;

(E) $\mathcal{E}(t, \phi(t), z(t)) + \int_s^t \int_\Omega \Delta(z, \dot{z})\mathrm{d}x\,\mathrm{d}t \le \mathcal{E}(s, \phi(s), z(s)) - \int_s^t \langle \dot{\ell}, \phi \rangle \mathrm{d}t.$

The flexibility of the energetic formulation allows for applications in continuum mechanics. The advantages are: (i) no derivatives of the solutions $(\mathrm{D}\phi, z)$ and of the constitutive functions ψ and Δ are required and (ii) there exists a natural incremental problem which reduces to minimizing $\mathcal{E}(t_k, \cdot, \cdot) + \mathcal{D}(z_{k-1}, \cdot)$.

All elastoplastic models with an associative flow rule can be put into our framework. In the case with finite strain we let $z = (P, p) \in \mathrm{SL}(3)\times\mathbb{R}$ and $\psi(F, P, p) = \widehat{\psi}(FP) + h(p)$. We argue that many standard material do not lead to coercive or quasiconvex problems and hence the incremental problem will not be solvable in general, which indicates localization or failure effects or leads to the formation of microstructure. Finally, we provide an example where existence can be shown.

Rigorous derivation of dimensionally reduced models in nonlinear elasticity

STEFAN MÜLLER (LEIPZIG)

(joint work with G. Frieseke (Warwick), R.D. James (Minessota), and later also with M.G. Mora (Leipzig))

We show how a hierarchy of two-dimensional theories, including the geometrically nonlinear Kirchhoff theory, the Föppl – von Kármán theory and its linearization can be rigorously derived (as suitable Γ-limits) of three dimensional nonlinear elasticity. Our approach is based on the scaling of the energy (in powers of the thickness). A key ingredient is the following nonlinear version of Korn's inequality.

Theorem *Let U be a bounded domain in $\mathbb{R}^n$, $n \geq 2$, with Lipschitz boundary. Then for every $v : U \to \mathbb{R}^n$ with $\nabla v \in L^2$ there exists a rotation $R \in SO(n)$ such that*

$$\int_U |\nabla v - R|^2 \, dx \leq C(U) \int_U \mathrm{dist}^2(\nabla v, SO(n)) \, dx \, .$$

This generalizes work of Fritz John (On rotation and strain, Comm. Pure Appl. Math., 1961). He assumed in addition that v is locally Bilipschitz, an assumption which does not follow from finiteness of the elastic energy.

The approach can also be extended to shells and rods.

Stress-strain behaviour of elastic bars with cohesive energy

GIANPIETRO DEL PIERO (FERRARA)

Equilibrium configurations for one-dimensional elastic bars in a hard device is considered. Equilibrium configurations are identified with stationary points of the energy, and the energy is assumed to consist of two parts, a bulk part depending on the deformation of the bar as a continuum, and an interfacial part, in which the "cohesive energy" is assumed to depend on the magnitude of the discontinuities in the axial displacement.

Among equilibrium configurations, of interest are those which are metastable, i.e., local minimizers of the energy. It is shown that the characterization of local minimizers can be reduced to the determination of the local minimizers of a sequence of finite-dimensional problems, each corresponding to a fixed number of discontinuities in the bar. Special forms of the interface energy lead to the reproduction of different well known classes of material behaviour: fracture (ductile and brittle), damage, and plastic deformation.

A proposal for the geometry and kinematics of multilattices, with application to the alpha-beta transition of quartz

MARIO PITTERI (PADOVA)

I provide an explicit, general framework for the kinematics of multilattices which is an alternative to one proposed earlier. The example given is the structural transition of beta-quartz, described by the 3-lattice model introduced by R.D. James (Vol. 3 of the IMA Volumes in Mathematics and its Applications, 1987). The analysis shows that, among others, there are two trigonal trapezohedral low-symmetry product phases, which are mutually orthogonal in a sense, and are both described by a 1-dimensional order parameter space. One of these is the alpha-phase as modelled by James. The other was obtained by Ericksen (J. of Elasticity, 63, 2001) as an outcome of the search for a third quartz phase, used to provide some rationale for the so-called incommensurate phase introduced in the physical literature to explain certain peculiarities of the alpha-beta transition. Here the geometry of the 3-lattice describing this new phase is given in detail.

Consistently ordered Extended Thermodynamics – application to light scattering experiments

DANIEL REITEBUCH (BERLIN)

Extended Thermodynamics is needed for rapidly changing fields with steep gradients. The new consistently ordered Extended Thermodynamics makes this fact explicit by assigning orders of magnitudes to the moments in terms of steepness of gradients. Application of such a theory to a light scattering experiment leads to a spectrum of the scattered light. Comparison with a reference spectrum allows to judge the quality of the theory. The most obvious choice for the reference spectrum is an experimental result. Such results are available, but not good enough for an accurate comparison. A powerful alternative for the reference spectrum is an exact solution of the Boltzmann equation with the BGK ansatz for the collision production, that was found by Yip & Nelkin [Phys. Rev, 1964]. The use of this reference solution allows a very accurate comparison between different theories of extended thermodynamics, and it turns out that the accuracy increases with an increasing number of field variables. Furthermore, the consistent theories seem to be more efficient than the ones used before, since they produce better results by use of a lesser number of variables.

Stability problems in fluid mechanics

SALVATORE RIONERO (NAPOLI)

Let

i) Ω be a Lebeasgue measurable domain;

ii) $\mathbf{u}(\mathbf{x},t)$, $(\mathbf{x},t)\in\Omega\times\mathbb{R}^+$, be a vector valued function such that $\mathbf{u}(\mathbf{x},t)\in L^p\Omega)$, $\forall\, t\geq 0$, $1\leq p\leq\infty$;

iii) $\tilde{\Omega}(\epsilon,t)\subset\Omega$ be the subdomain such that $\mathbf{x}\in\tilde{\Omega}(\epsilon,t)\Rightarrow|\mathbf{u}(\mathbf{x},t)|>\epsilon$, ϵ being a positive constant;

iv) $\tilde{\mu}(\epsilon,t)$ be the Lebesgue measure of $\tilde{\Omega}(\epsilon,t)$.

It is shown that – both in the cases Ω bounded, Ω unbounded – the inequality

$$\tilde{\mu}(\epsilon,t)\leq\epsilon^{-p}\,||\mathbf{u}(\mathbf{x},t)||_p^p$$

holds ($||\,||_p$ being the $L^p(\Omega)$-norm) and that the conditions guaranteeing the attractivity with respect to the $L^p(\Omega)$-norm of a basic flow $\mathbf{U}$ of a dynamical system, guarantee the attractivity of $\mathbf{U}$ with respect to the $L^\infty(\Omega)$-norm. When the perturbations to the basic flow $\mathbf{U}$ verify an energy relation like the one verified by the weak solutions of the Navier-Stokes equations, a methodology for obtaining the attractivity with respect to the $L^\infty(\Omega)$-norm, in the case Ω unbounded, is observed. An application to the nonlinear diffusion of a gas in an unbounded porous domain, in the case of the Dirichlet problem, is studied.

Wave speeds in Extended Thermodynamics

TOMMASO RUGGERI (BOLOGNA)

The first motivation of Extended Thermodynamics was to solve the paradox of infinite velocity for the disturbances that are present in the heat equation and in general in the case of continuum theories with Fourier, Navier-Stokes constitutive equations.

In this review presentation first we introduce the closure method of modern Rational Extended Thermodynamics for the Moment System associated to Boltzmann equation and then we obtain a lower bound estimate for the maximum wave speed for a generic moment system truncated at the tensorial order n. In particular in the case of classical rarefied gas we prove that

$$\frac{\lambda_{max}}{c_s} \geq \sqrt{\frac{6}{5}\left(n-\frac{1}{2}\right)}\,, \tag{1}$$

where c_s is the sound velocity and λ_{max} is the maximum characteristic speed. The index n is related to the number of moments through the relation

$$N = \frac{1}{6}(n+1)(n+2)(n+3)\,.$$

From (1) we deduce that λ_{max} becomes unbounded when the number of moments tends to infinity. Therefore we arrive to the conclusion that for all finite number of moments λ_{max} is finite (symmetric hyperbolic system), but in the limit of $n \to \infty$, $\lambda_{max} \to \infty$!!

An analogous, but with more complicated inequalities, can be done in the relativistic framework:

$$1 \leq \frac{\lambda_{max}^2}{c^2} \leq \frac{2n-1}{\gamma}\frac{K_{n+1}(\gamma)}{K_{n+2}(\gamma)}\,,$$

where c is the light velocity, K_n is the Bessel function and $\gamma = \dfrac{mc^2}{KT}$ (K is the Boltzmann constant and T is the absolute temperature). Therefore when $n \to \infty$, $\lambda_{max} \to c$. This last result can be obtained also in the case of degenerate gas, as Fermi and Bose gas.

On deformation induced anisotropy in the context of large strain elasto-plasticity of metallic foams

INGO SCHMIDT (DARMSTADT)

Advances in manufacturing technology have made metallic foams a potential candidate for a number of engineering applications ranging from energy absorption - to load bearing sandwich structures. Due to their specific microstructure and their capability of undergoing very large – usually compressive – strains, highly porous metallic foams develop pronounced anisotropies in both elastic and plastic properties.

The presentation discusses some aspects of an internal-variable framework of plasticity based on the multiplicative decomposition of the deformation gradient F into an elastic and a plastic part $F = F_e F_p$, which is shown to result from the assumption of the existence of an elastic range. It is shown that the use of tensorial internal variables renders the free energy invariant with respect to changes in the orthogonal part of F_p and that this invariance leads to a symmetric stress measure as the variable dual to the "plastic strain rate " $\dot{F}_p F_p^{-1}$. Based on the concept of a representative volume element, a computational strategy is presented which allows for the simulation of a (model-) material response to

arbitrary straining paths, including in particular ones that are not accessible in usual experimental setups. The evolving elastic stiffnesses and yield surfaces are computed for selected straining paths and the normality hypothesis is verified. It is further shown that elastic and plastic anisotropies are closely related to each other.

Nonlinear stability in penetrative convection

BRIAN STRAUGHAN (DURHAM)

The phenomenon of penetrative convection in a fluid or a saturated porous medium is explained. Novel effects which are due to the penetrative effect are displayed. For example, with two salt fields and a temperature field it is shown oscillatory and stationary convection can occur at the same critical Rayleigh number, but different wavenumbers. An interesting array of streamline patterns is obtained for penetrative convection in water overlaying a saturated porous medium. Finally, linear and unconditional nonlinear stability thresholds are derived for a model due to R. Krishnamurti. This model achieves a stable layer which is heated internally by radiation due to a sodium lamp.

Regularizations of Grad's 13 moment equations – derivation and linear stability

HENNING STRUCHTRUP (VICTORIA)

A new method for closure of moment equations in kinetic theory is proposed, which can be considered as a combination of the method of moments of Grad, and the Chapman-Enskog method. This method is used to give an alternative closure of Grad's 13 moment equations. The new closure adds terms of Super-Burnett order (3rd order in the Knudsen number) to the usual Grad equations. The resulting system of equations contains parabolic terms, and is thus of different character than the Grad equations which are hyperbolic. A Chapman-Enskog-like expansion of the equations reveals that the new set of equations indeed agrees with the Boltzmann equation up to the Super-Burnett level. However, other than the Burnett and Super-Burnett equations, the new equations are linearly stable for disturbances of arbitrary wave length or frequency.

Applications of the equations with comparison to experiments are discussed in Torrilhon's talk.

A new continuum theory of crystals incorporating microscopic thermal vibration and its applications to wave propagation phenomena

MASARU SUGIYAMA (NAGOYA)

Microscopic basic equations for analyzing nonequilibrium phenomena in 3-dimensional enharmonic crystals lattices at finite temperatures are self-consistently derived from the Liouville equation by adopting both independent particle approximation and Gaussian approximation.

Macroscopic basic equations are also derived from the microscopic basic equations by the continuum approximation. The equations may also be regarded as new equations for finite deformation continuum theory incorporating microscopic thermal vibration of constituent atoms.

By using the microscopic and macroscopic basic equations, linear waves in crystals are analyzed and discussed with special attention to the cases at high temperatures near the melting point.

Regularization of Grad's 13-moment-equations – applications

MANUEL TORRILHON (ZÜRICH)

Recently, a hybrid gas kinetic approach (presented here in the talk of H. Struchtrup) yielded a new system of field equations, called regularized 13-moment-equations (R13), supposed to describe dilute gas flows. This talk presents results of the new system applied to the problems of sound waves, light scattering and shock waves. In all cases the R13-system shows satisfying agreement with measurements, DSMC-simulations and exact solutions, respectively. Furthermore the results are found to be superior to results of classical theories like the system of Navier-Stokes-Fourier or Grad's 13-moment-equations. The R13-shock profile is smooth for any Mach number. By investigating the positivity of Grad's distribution function inside the shock we also discuss the validity range of the new theory.

Algebraic description of dissipative systems

LUKASZ A. TURSKI (WARSAW)

I have presented a novel approach to the description of the dissipative systems dynamics which is based on extension of the concepts known from symplectic dynamics. This method, called metriplectic dynamics, combines "Poisson brackets" with "dissipative brackets". Formal presentation of the theory was illustrated on examples from various fields of physics: fluid mechanics, spin dynamics and wave mechanics.

Biaxial order parameters in nematic liquid crystals

EPIFANIO G. VIRGA (PAVIA)
(joint work with G.E. Durand (Paris) and A.M. Sonnet (Glasgow))

By use of two order tensors and a simplified mean-field model, we recover the classical sequence of phases: isotropic-uniaxial-biaxial, in a nematogenic material composed of intrinsically biaxial molecules. Each phase is practically described by a single scalar order parameter, instead of the two needed in more general models. This simplified model led us to a new expression of the free energy, which has the potential to describe better the diverse order reconstructions observed experimentally.

Micro-macrotransitions for granular materials. Estimations of porosity dependence

KRZYSZTOF WILMANSKI (BERLIN)

A thermodynamic derivation of a generalized Biot's model for porous materials is presented and some of its acoustic properties are discussed. These are used in the evaluation of in situ experiments in order to find a dependence of macroscopic properties from the porosity. The transition from microscopic to macroscopic properties is performed by use of simple tests proposed by Biot and Willis. A rational scheme for this transition is developed.

Modelling materials with a triple point – an alternative approach to Landau theory

JOHANNES ZIMMER (PASADENA)
(joint work with P. Dondl (München))

A class of energy functions is derived for the triple point of zirconia (ZrO_2), where tetragonal, orthorhombic (orthoI) and monoclinic phases are stable. After presenting a simple framework to deal with the tetragonal-orthorhombic-monoclinic symmetry, an energy is fitted to the experimental data of zirconia. Instead of the traditional Landau ansatz (understood in the sense that the energy is constructed of polynomials), we use the orbit space method. This enables us to deal in a very simple way with the symmetry constraints. Moreover, in this framework it is easy to use a modular approach to derive an energy function.

Edited by Ioana Luca

Participants

Prof. Dr. Hans-Dieter Alber
alber@mathematik.tu-darmstadt.de
Fachbereich Mathematik
TU Darmstadt
Schloßgartenstr. 7
D–64289 Darmstadt

Prof. Dr. Hans Wilhelm Alt
alt@iam.uni-bonn.de
Institut für Angewandte Mathematik
Universität Bonn
Wegelerstr. 6
D–53115 Bonn

Prof. Dr. Romesh C. Batra
rbatra@vt.edu
ESM Department
M/C 0219
VPI & SU
220 Norris Hall
Blacksburg, VA 24061 - USA

Prof. Dr. Victor Berdichevsky
vberd@eng.wayne.edu
res0hupd@verizon.net
College of Engineering
Mechanical Engineering Department
Wayne State University
2138 Engineering Bldg.
Detroit MI 48202 - USA

Prof. Dr. Andrea Braides
braides@mat.uniroma2.it
Dipartimento di Matematica
Universita di Roma
Tor Vergata
V.della Ricerca Scientifica, 1
I-00133 Roma

Prof. Dr. Yann Brenier
brenier@dmi.ens.fr
brenier@math.unice.fr
brenier@ann.jussieu.fr
Laboratoire J.A. Dieudonné
Université de Nice
Sophia Antipolis
Parc Valrose
F-06108 Nice Cedex 2

Prof. Dr. Martin Brokate
brokate@appl-math.tu-muenchen.de
Zentrum Mathematik
TU München
D–85747 Garching bei München

Prof. Dr. Wolfgang Bürger
buerger@math.uni-karlsruhe.de
Universität Karlsruhe
Fakultät für Mathematik
D–76128 Karlsruhe

Prof. Dr. Paolo Cermelli
cermelli@dm.unito.it
Dipartimento di Matematica
Universita degli Studi di Torino
Via Carlo Alberto, 10
I-10123 Torino

Dr. Sergio Conti
conti@mis.mpg.de
Max-Planck-Institut für Mathematik
in den Naturwissenschaften
Inselstr. 22 - 26
D–04103 Leipzig

Prof. Dr. Gianpietro Del Piero
gdpiero@ing.unife.it
Dipartimento di Ingegneria
Universita di Ferrara
Via Saragat, 1
I-44100 Ferrara

Dr. Wolfgang Dreyer
dreyer@wias-berlin.de
Weierstraß-Institut für
Angewandte Analysis und Stochastik
im Forschungsverbund Berlin e.V.
Mohrenstr. 39
D–10117 Berlin

Prof. Dr. Sergey Gavrilyuk
sergey.gavrilyuk@univ.u-3mrs.fr
Laboratoire de Modélisation en
Mécanique et Thermodynamique
Université Aix-Marseille III
Avenue Escadrille Normandie-N.
F-13397 Marseille Cedex 20

Prof. Dr. George Herrmann
g.herrmann@dplanet.ch
Ortstr. 7
CH-7270 Davos-Platz

Dr. Yongzhong Huo
yzhuo_cd@yahoo.com
Shanghai Institute of Ceramics
Chinese Academy of Sciences
1295 Ding-Xi Road
Shanghai 200050 - CHINA

Prof.Ph.D. Kolumban Hutter
hutter@mechanik.tu-darmstadt.de
Institut für Mechanik
Technische Hochschule Darmstadt
Hochschulstr. 1
D–64289 Darmstadt

Dr. Michael Junk
junk@mathematik.uni-kl.de
Fachbereich Mathematik
Universität Kaiserslautern
Erwin-Schrödinger-Straße
D–67653 Kaiserslautern

Dr.Ing. Marc Kamlah
kamlah@imf.fzk.de
Institut für Materialforschung II
Forschungszentrum Karlsruhe
Postfach 3640
D–76021 Karlsruhe

Dipl.-Ing. Oliver Kastner
Kastner@thermodynamik.tu-berlin.de
Inst. für Verfahrenstechnik
FG Thermodynamik
Techn. Universität Berlin
Fasanenstr. 90
D–10623 Berlin

Prof. Dr. Reinhold Kienzler
rkienzler@uni-bremen.de
IW3
Universität Bremen
Postfach 330440
D–28334 Bremen

Prof. Dr. Robin John Knops
r.j.knops@hw.ac.uk
Dept. of Mathematics
Heriot-Watt University
Riccarton-Currie
GB-Edinburgh, EH14 4AS

Prof. Dr. Gilberto M. Kremer
kremer@fisica.ufpr.br
Departamento de Fisica
Universidade Federal do Parana
Caixa Postal 19081
Curitiba 81531-990 - BRAZIL

Prof. Dr. Meinhard Kuna
meinhard.Kuna@imfd.tu-freiberg.de
TU Bergakademie Freiberg
Institut für Mechanik und
Fluiddynamik
Lampadiusstr. 4
D–09596 Freiberg

Prof. Dr. Khanh Chau Le
chau@am.bi.ruhr-uni-bochum.de
Lehrstuhl für Allgemeine Mechanik
Ruhr-Universität Bochum
Universtitätsstr. 150
D–44801 Bochum

Ioana Luca
iolucaro@yahoo.com
Departement of Mathematics
Polytechnical University of
Bucharest
Splaiul Independentei 313
Bucharest - Romania

Prof. Dr. Stephan Luckhaus
luckhaus@mathematik.uni-leipzig.de
luckhaus@mis.mpg.de
Fakultät für Mathematik/Informatik
Universität Leipzig
Augustusplatz 10/11
D–04109 Leipzig

Prof. Dr. Alexander Mielke
mielke@mathematik.uni-stuttgart.de
Institut für Analysis, Dynamik
und Modellierung
Universität Stuttgart
Pfaffenwaldring 57
D–70569 Stuttgart

Prof. Dr. Ingo Müller
im@thermo08.pi.tu-berlin.de
im@thermodynamik.tu-berlin.de
Inst. für Verfahrenstechnik
FG Thermodynamik
Techn. Universität Berlin
Fasanenstr. 90
D–10623 Berlin

Prof. Dr. Stefan Müller
Stefan.Mueller@mis.mpg.de
sm@mis.mpg.de
Max-Planck-Institut für Mathematik
in den Naturwissenschaften
Inselstr. 22 - 26
D–04103 Leipzig

Prof. Dr. Mario Pitteri
pitteri@dmsa.unipd.it
Dipartimento di Metodi e Modelli
Matematici
Universita di Padova
Via Belzoni, 7
I-35131 Padova

Daniel Reitebuch
daniel@thermodynamik.tu-berlin.de
Inst. für Verfahrenstechnik
FG Thermodynamik
Techn. Universität Berlin
Fasanenstr. 90
D–10623 Berlin

Prof. Dr. Salvatore Rionero
rionero@unina.it
Dipartimento di Matematica
Universita di Napoli
Via Mezzocannone, 8
I-80134 Napoli

Prof. Dr. Tommaso Ruggeri
ruggeri@ciram.unibo.it
Dipart. di Matematica- C.I.R.A.M.
Universita di Bologna
Via Saragozza, 8
I-40123 Bologna

Dr.-Ing. Ingo Schmidt
i.schmidt@mechanik.tu-darmstadt.de
Institut für Mechanik
Technische Universität Darmstadt
Hochschulstr. 1
D–64289 Darmstadt

Prof. Dr. Brian Straughan
brian.straughan@durham.ac.uk
Dept. of Mathematical Sciences
The University of Durham
Science Laboratories
South Road
GB-Durham, DH1 3LE

Prof. Dr. Henning Struchtrup
struchtr@uvic.ca
Dept. of Mechanical Engineering
University of Victoria
Victoria, BC V8W 3P6 - Canada

Prof. Dr. Kurt Suchy
0211203410@t-online.de
Institut f. Theoretische Physik II
Universität Düsseldorf
Universitätsstr. 1
D–40225 Düsseldorf

Prof. Dr. Masaru Sugiyama
sugiyama@system.nitech.ac.jp
Dept. of Systems Engineering
Nagoya Institute of Technology
Gokiso-cho
Showa-ku
Nagoya 466-8555 - Japan

Manuel Torrilhon
manuel@math.ethz.ch
Seminar für Angewandte Mathematik
ETH-Zentrum
Rämistr. 101
CH-8092 Zürich

Prof. Dr. Lev Truskinovsky
trusk@aem.umn.edu
Department of Aerospace Engineering
and Mechanics
University of Minnesota
110 Union Street S. E.
Minneapolis, MN 55455 - USA

Prof. Dr. Lukasz A. Turski
laturski@cft.edu.pl
Center for Theoretical Physics of
the Polish Academy of Sciences
Dept. of Nat. Sc. and Mathematics
Cardinal Wyszynski University
Warsaw 02-668 - Poland

Prof. Dr. Epifanio G. Virga
virga@ian.pv.cnr.it
Dipartimento di Matematica
"F.Casorati"
Universita di Pavia
via Ferrata 1
I-27100 Pavia

Prof. Dr. Krzysztof Wilmanski
wilmansk@wias-berlin.de
Weierstraß-Institut für
Angewandte Analysis und Stochastik
im Forschungsverbund Berlin e.V.
Mohrenstr. 39
D–10117 Berlin

Dr. Giovanni Zanzotto
zanzotto@ulam.dmsa.unipd.it
Dipartimento di Metodi e Modelli
Matematici
Universita di Padova
Via Belzoni, 7
I-35131 Padova

Dr. Johannes Zimmer
zimmer@caltech.edu
Division of Engineering and
Applied Sciences; MS 104-44
California Institute of Technology
Pasadena, CA 91125 - USA