Tagungsbericht 36/1996

Thermodynamische Materialtheorien

22.9. - 28.9.1996

The meeting was organized by Prof. Wolfgang Bürger (Karlsruhe), Prof. Karl-Heinz Hoffmann (München), Prof. Ingo Müller (Berlin) and Prof. Jürgen Sprekels (Berlin).

The topics treated in the conference covered mathematical and physical aspects of thermodynamic constitutive theories and phase transitions.

Contributions to the field of constitutive theories included aspects of hyperbolic systems, particularly those of extended thermodynamics, liquid crystal behavior, the treatment of porous media and glaciers. Phase transitions have been treated in several presentations on shape memory behavior, microstructures in super alloys as well as Stefan problems and hysteretic behavior.

An overview of the individual contributions can be found in the subsequent collection of abstracts.

On the Existence of Entropy in Non-Equilibrium

H.W. Alt

We present an evolution principle in an abstract setting, which can be used to prove the existence of an entropy. It is shown that for an ordinary differential equation this evolution principle is equvalent to Caratheodory's inaccessibility axiom and therefore to the existence of entropy. Further, a first order system is considered. It is shown that in special cases (a hyperbolicity assumption) the existence of an entropy follows from the above principle.

I thank I. Müller who put my attention to the problem here in Oberwolfach in May 1995.

Mathematical Modeling of Charge Carrier Transport in Semiconductors: Problems and Perspectives

A.M. Anile

The semiclassical Boltzmann equation (BTE) for charged carriers in semiconductors is briefly introduced and some related important mathematical problems are highlighted. The diffusion limit and the hydrodynamical limit are discussed and their foundations are critically reviewed. A consistent approach is proposed for the hydrodynamical models based on the exponential moments method for solving the BTE (physically equivalent to the principles of extendet hydrodynamics).

Relaxation in shape-memory alloys.

K. Bhattacharya

A variety of relaxation phenomena such as the stabilization of martensite, rubber-like behavior, evolving hysteresis loops and stabilization of interfaces have been observed in various shape-memory alloys. These effects adversely impact technological applications. Despite a great deal of experimental evidence, there is no consensus on the mechanism. However, there is universal agreement on certain fundamental aspects of these phenomena. Based on these areas of agreement, we propose a phenomenological, but predictive, model. This model is based on the framework of thermoelasticity augmented with an internal variable,and yields a very interesting class of ordinary differential equations witha discontinuous forcing function. We show that the model reproduces the experimental observations remarkably well and use this model to propose new experiments in order to clarify longstanding issues.

Moment Equations in the Kinetic Theory of Gases and Wave Velocities

G. Boillat

We consider the evolution system for N moments of the Bolzmann equation and we require the compatibility with an entropy law that implies that the distribution function $f(\mathbf{x}, t, \mathbf{c})$ depends only on a single polinomial variable χ in $\mathbf{c}$. Then it is possible to construct the generator, such that the system assumes in the mainfield a symmetric hyperbolic form. For an arbitrary $f(\chi)$ the system obtained maximizes the entropy density. If we impose that our entropy coincides with the usual one of non-degenerate gases we obtain a particular exponential function for $f(\chi)$ already found by Dreyer. For these results the behavior of the characteristic wave velocities for increasing number of moments is studied and we show that in the classical theory the maximum velocitiy increases and tends to infinity while in the relativistic case the wave and shock velocities are bounded by the speed of light.

Nonlinear Kinematic Hardening

M. Brokate

We consider a certain class of elastoplastic rate independent stress-strain laws, namely those of kinematic hardening type, which include the models of Prager, Armstrong and Frederick, Chaboche and Mróz. We prove wellposedness in the space of absolutely continuous functions both for the stress-controlled and the strain-controlled case under appropriate restrictions of the domain of definition.

Some Observations in Elementary Geometry, Toy & Everyday Physical Phenomena

W. Bürger

Starting with the taxicab geometry of Karsruhe and Max Bill's family of half sphere twins which decorate the courtyard of the mathematics department of the university there, the lecture dwelt upon several simple but nonetheless surprising phenomena, among others the balance of a ruler on two fingers, the paper clip top made from one single wire, the butter toast catastrophe, some toilet paper problems, and a theory of flying kites which allows the rising of kites to be calculated. It was shown how the work in offices can be made more pleasant by building business office boomerangs which are difficult to get rid off by throwing. Emphasis was laid on the importance of ORIGAMI (paper folding) for the teaching of elementary geometry, and it was demonstrated how any angle in the plane can be trisected exactly by only three straight folds.

Stress and Heat Flux in Non-inertial Reference Frames

C. Cercignani

Chapman and Cowling noted that, in a non-inertial frame of reference, this stress tensor may depend on the angular velocity of the frame and obtained an approximate expansion in which the total pressure was found to be negative for sufficiently strong angular velocities (as consequence of the approximation). More than thirty years later, in 1972, Müller showed that the heat flux depends on ω too. In this talk, based on research done in collaboration with Paolo Biscari, we compute the heat flux and the stress tensor in a gas assuming that $\omega\tau$, where τ is the microscopic collision time, is non-negligible, even when τ is small. Our results confirm those of Müller for small angular velocities and show that, even when is large, the inertial effects always reduce the heat flux and the magnitude of the stress tensor. Since τ is usually very small, the effects we predict are not easy to observe, unless we are able to put our system into a very strong rotation. Granular materials may be a good example to observe these inertial effects: In these systems, even if we usually are at high densities, τ is much higher than in gases, since the much greater size of the particles (here grains, rather than molecules) increases the average collision time, an thus a much smaller ω is required to make $\omega\tau$ significant. We have not been able, so far, to develop a theory holding from low to high values of ω which can be applied to the same observed experimental apparatus. This is important to judge the objectivity of the theory and will be our next concern.

Evolving Microstructure of Single Crystal Superalloys

W. Dreyer

Because of their favorable properties at high temperatures two phase nickel-based single crystal superalloys have been used for many years as turbine blade material. In service the blades are subject to complex thermal and mechanical loading conditions which change between low and high temperature as well as between tension, compression and torsion. In the virginal superalloy, the ordered γ'-phase precipitates within the disordered γ-phase resulting in an almost periodic pattern of γ'-cuboids. The crystal structure of both phases is face centered cubic. However, the lattice parameters of both phases are different which leads to the formation of eigenstresses.

As a consequence of the eigenstresses and of the aforementioned loads a change of the morphology of the metastable $(\gamma - \gamma')$-structure will occur.

At a given temperature T, and for given external load $\mathbf{f}$, we describe the thermomechanical microstate of the superalloy by the fields of strain, concentration of alloy elements and by the order parameter that measures their distribution over the lattice sites. The field equations for these fields rely on Cahn-Hilliard type equations. It is crucial to take into account the different elastic properties

of the phases.

The figure shows the evolving microstructure for the special case that the vertical load axis deviates by 12° to the (001)-crystal axis. The change of the intitial state shown in the left picture, to the rafted structure is due to a tensile load and lasts at 950°C about 200 hours.

Constitutive Theories of Shape Memory Alloys Related to Microstructure

F. Falk

The shape memory effect is due to a martensitic phase transition deforming the crystal lattice. Because of elastic misfit of the product phase within the matrix of the parent phase inhomogeneous microstructures arrays at two different length scales. As a consequence, the deformation to be observed differs on different length scales and one thoroughly has to discriminate between different levels of description. For shape memory alloys the deformation on each level are discussed. Moreover, constitutive theories covering the whole range from microscopic dimensions up to macroscopic polycrystals are reviewed and their interrelations are discussed. Special emphasis is given to Landau and Ginzburg-Landau theories.

The Principle of Virtual Power and the Power of Internal Forces

M. Frémond

In continuum solid mechanics the power of the internal forces is chosen as $\int \sigma D\left(\vec{V}\right) d\Omega$ where σ is the stress tensor and $D\left(\vec{V}\right)$ is the strain rate tensor. Are there other choices which are useful for mechanics?

1. Let us consider a mixture of sand and long textile fibres (used to make very effective retaining walls in civil engineering). The fibres apply actions at a distance. Thus, the power of the interior forces

$$-\int \sigma D\left(\vec{V}\right) d\Omega + \int\int 2M\left(x,y\right)\left(\vec{x}-\vec{y}\right)\left(\vec{V}\left(x\right)-\vec{V}\left(y\right)\right) dxdy$$

takes care of the distance actions applied by the fibres ($M\left(x,y\right)$ is a new gereralized interior force (the intensity of an interaction force)).

2. Damage, for instance damage of concrete, results from microscopic motions. We decide to take into account the power of these microscopic motions and at the same time to remain at the macroscopic level. The volume fraction of undamaged material is introduced $(\beta(x,t))$. The power

$$-\int \sigma D\left(\vec{V}\right) d\Omega - \int \left\{\beta\dot{\beta} + M\, grad\, \dot{\beta}\right\} d\Omega$$

takes into account the microscopic motions.

In case (1) and (2), partial differential equations describe the evolution of structures

$$\Delta\vec{u} - \int \left\{(\vec{x}-\vec{y})\left(\vec{u}(x)-\vec{u}(y)\right)\right\}^{+}(\vec{x}-\vec{y})\, dy + \vec{f} = 0, \quad +B.C.$$

where $\{x\}^{+} = \sup\{0,x\}$ (the fibres have a unilateral behavior!), $\vec{f}$ are the body forces,

$$\begin{aligned} div\,(\beta\, grad\,\vec{u}) + \vec{f} &= 0 \\ \dot{\beta} - \Delta\beta - w + \frac{1}{2}(grad\,\vec{u})^2 + \partial I(\beta) + \partial I_{-}\left(\dot{\beta}\right) &\rightarrow 0, \quad +I.C., +B.C. \end{aligned}$$

where I is the indicator function of $[0,I]$ and I of $\Re^n$ $(n>0)$.

3. The system made of a point and a fixed plane is deformable because the distance of the point to plane changes. Because it is deformable, there are interial forces which are defined by their virtual work

$$-\beta^{int}\frac{\vec{V}^{+}(t)+\vec{V}^{-}(t)}{2} - \int_{t_1}^{t_2} R(\tau)\, V(\tau)\, d\tau$$

The velocity is a bounded variational function. $\vec{V}^{+}$ is the right limit and $\vec{V}^{-}$ the left value at a discontinuity point. The resulting evolution equation is a differential inclusion.

A Continuum Approach to Model Induced Anisotropy in Glaciers and Ice sheets

K. Hutter

The talk presents a formulation of a continuum model for so-called (stress or deformation) induced anisotropy in natural ice which, unlike computer based models, can be incorporated in (numerical) simulations of large ice masses to account for the effects of this process on the flow of these bodies in a physically reasonably acceptable fashion. To do this, natural ice is treated as rigid-(elastic), non-linear viscous material which can develop transverse isotropic behavior - (thus accounting for the simplest kind of induced anisotropy in natural ice masses), - where the degree of such anisotropy at each point is controlled

by the distribution of crystal glide plane orientations there. This distribution is described by a so-called distribution function, for which an evolution relation can be derived. The central constitutive assumption of this formulation relates this distribution to the "structure" tensor representing the transverse isotropy of the material. We present a few examples under shearing deformations and also show that the model predicts isotropic behavior and recovers the classical behavior at a point, when the distribution function of crystal glide plane orientations is uniform there.

Numerical Solutions for Dynamic Formation of Phase Mixtures

I-Shih Liu

One-dimensional motion of a body capable of phase transitions is often described by the usual equations of elasticity with a non-monotone stress-strain relation. We give a numerical treatment for a Riemann problem of an elastic bar based on the sequence of solutions for a rate type viscoelastic problem as the relaxation parameter tends to zero. It is found that approximate solutions may consist of numerous successive stationary jump discontinuities in strain, thus interpreted as phase mixtures. Such jump discontinuities in the vanishing relaxation limit become intense oscillations, which we call oscillation waves. It gives rise to the so-called measure-valued solutions for which the mean values of the state variables and the fluxes, based on the probability measures induced by the approximate solutions, satisfy the system in the sense of distributions. Numerical determination of the mean values and the verification of Rankine-Hugoniot conditions are shown for initial Riemann data inside the region of phase transitions.

The Effect of Geometric Shape on Behavior in Saint Venant's Principle

R.J. Knops

This account of a joint study with L.E. Payne is prompted by the realization that although the mathematical investigation of Saint Venant's principle should be within the context of the Phragmen-Lindelöf principle, the former, formulated originally for cylindrical regions yields exponential asymptotic decay behavior of the solution, while the latter principle, at least in its classical form, was established for sectorial regions and admits algebraic (alternative) behavior. Geometry obviously affects behavior.

Additionally, however, behavior is also affected by the average measures of the solution. For example, the method adopted here employs the surface energy flux taken over plane spherical and more general surfaces (for which a first order differential inequality is derived and discussed) and thus might be expected to

affect the descriptions of the solution's behavior.

These interrelationships are here illustrated by several examples for sectorial regions (e.g., cones in $\Re^3$, the half-space, exterior regions and the whole space); and the thick plate with plane faces, including the quarter space. For simplicity, only linearized elasticity is discussed under appropriate homogeneous Dirichlet boundary conditions, but other theories and boundary conditions can also be considered.

These examples suggest that those regions for which at least one-dimension remains bounded (e.g. cylinders and thick plates) admit exponential alternative behavior for the solution, while for regions for which all three dimensions become unbounded (e.g. cones in $\Re^n$, $n = 2, 3$) admit algebraic alternative behavior. The manifold over which the solution is averaged appears not to have any affect.

On the Dynamic Pressure in Relativistic Gases

G. M. Kremer

Based on extended thermodynamics of a single relativistic gas it is shown that the dynamic pressure is due to an expansion proportional to the divergence of the four-velocity of order $1/c^4$, and a heating proportional to the divergence of the heat flux of order $1/c^2$, which provides the leading contribution to the dynamic pressure.

For a chemically reacting non-diffusive binary mixture it is shown, that even a non-relativistic mixture of gases has a non-vanishing bulk viscosity, which is determined by the mass defect (or the heat of reaction). Moreover, the thermal conductivity is also affected by the heat of reaction.

Thermodynamics of Hysteresis

P. Krejčí

We propose a hysteretic model of a temperature-strain-stress constitutive law for thermoelastoplastic materials which is compatible with the second principle of thermodynamics. We derive the expressions for the hysteresis free energy and entropy operators and prove the existence of solutions to an initial-boundary value problem for the corresponding equation of motion coupled with the energy balance equation governing the uniaxial dynamical behavior of a thermoelastoplastic solid.

Some Flow Effects in a Continuum Theory for Smectic C Liquid Crystals

F.M. Leslie

In a recent paper, Leslie, Stewart and Nakagawa propose a continuum theory for smectic C liquid crystals that employs two assumptions to simplify the

resulting theory, on that the layers remain of constant thickness and the second that the tilt of the mean molecular alignment with respect to the layer normal remains fixed. Such a theory although restricted in its range of applicability is likely to be useful in modeling behavior in certain display devices.

After a brief summary of the theory this paper reviews progress in analyses of flow effects employing the theory. Firstly, it shows that the theory can predict flow alignment when the layers are parallel to the bounding plates, as observed in practice. Also, it discusses the response to shear flow in some detail including transverse flow effects for this particular case. Finally, a solution is presented describing a "backflow effect" when an initially distorted alignment relaxes, thus clearly demonstrating the need to include flow in transient behavior in display devices.

Thermomechanical Theory of Martensitic Phase Transitions in Inelastic Materials

V. Levitas

A general thermomechanical theory of phase transitions (PT) in elastoplastic materials is presented. The PT criterion and extremum principle for the determination of all unknown parameters are derived. A number of boundary-value problems are solved analytically and numerically:

- PT in a thin layer under applied normal and shear stresses,
- PT under compression and shear in Bridgeman anvil,
- PT in a spherical inclusion within elastoplastic cylindrical matrix (coherent and non-coherent interface, interface with fracture),
- propagation of non-coherent interfaces,
- progress of PT region in elastic and elastoplastic specimen.

Stefan Problems and the Maximal Entropy Condition

S. Luckhaus

An interpretation is given for the implicit time discretization for the classical Stefan problem:

$$\partial_t (u + \chi) - \Delta u = 0 \qquad \chi \in H(u)\,, \quad H \text{ the Heaviside function,}$$

which easily extends to Gibbs-Thomson laws for the phase change. This form of the discretization of (1) is:

$$\int (e - \chi)^2 + \frac{1}{h} \|e - e(t-h)\|^2_{H^{-1}} \to \min \quad \text{under the constraint } 0 \le \chi \le 1$$

$[e = u + \chi \qquad -$ the energy density$]$

In the Gibbs-Thomson law $\chi \in H(u)$ is replaced by $u \sim$ mean curvature of the phase interface. The corresponding implicit time discretization is

$$\int \frac{(e-\chi)^2}{2} + \alpha \int |\nabla \chi| + \frac{1}{2h} \|e - e(t-h)\|^2_{H^{-1}} \to \min \quad \text{under } \chi(1-\chi) \equiv 0$$

This can also be extended to systems of heat and mass diffusion in alloys, which in each phase can be written as

$$\partial_t (e, c) = \nabla (A_\alpha \nabla \vec{u}), \qquad \vec{u} = -\partial S_\alpha$$

where $S_\alpha(e, c)$ the entropy density in each phase is assumed to be convex. The corresponding generalization is:

$$S - \sum_\alpha \chi_\alpha S_\alpha (e, c) + \sum_{\alpha,\beta} \gamma_{\alpha\beta} (|\nabla \chi_\alpha| + |\nabla \chi_\beta| + |\nabla (\chi_\alpha + \chi_\beta)|) + \frac{1}{2h} < |\delta(e, c), \delta(e, c)\rangle$$

minimal for $\chi_\alpha (1 - \chi_\alpha) \equiv 0, \quad \sum \chi_\alpha \equiv 1.$

$$L\,\vec{u} = div \left(\sum A_\alpha \chi_\alpha (t-h) \nabla \vec{u} \right), \quad \delta(e, c) = (e, c) - (e(t-h), c(t-h))$$

under additional conditions [esp. $\left|\partial S_\alpha^{-1}(\vec{u}) - \partial S_\beta^{-1}(\vec{u})\right| \geq c > 0$] convergence is shown to:

$$\partial_t (e, c) = div \left(\sum A_\alpha \chi_\alpha \nabla \vec{u} \right), \quad \chi_\alpha \vec{u} = -\chi_\alpha \partial S_\alpha (e, c)$$

mean curvature of the interface between the α- and β-phase proportional to

$$\partial S_\alpha^* (\vec{u}) - \partial S_\beta^* (\vec{u}) = \partial S_\alpha^{-1} (\vec{u}) - \partial S_\beta^{-1} (\vec{u}).$$

Symmetry-breaking Transformations and Transformation Twins

M. Pitteri

The investigation of microstructures is largely based on the knowlegde of the transformation twins that are possible for a crystal undergoing a symmetry-breaking, diffusionless phase transition. In order to have a complete description of this phenomenon, we suitably localize the general invariance group $GL(3, \mathbf{Z})$ of a simple lattice by restricting the attention to a suitable neighborhood N_C of some lattice C, the latter beeing assumed to have maximal symmetrie for simplicity (and completeness). If $\mathbf{E}_a$ are basis vectors for the lattice having metric C, for any metric $\bar{C}$ in N_C the lattice group (arithmetic holohedry) $L\left(\bar{\mathbf{E}}_a\right) \subseteq L(\mathbf{E}_a)$ and two metrices $\bar{C}$, $\hat{C}$ have the same lattice group if and only if the have the

same holohedry: $P\left(\bar{\mathbf{E}}_a\right) = P\left(\hat{\mathbf{E}}_a\right)$. Thus all the possible symmetry-breaking transitions in N_C are analyzed by studying the holohedral subgroups of $P\left(\mathbf{E}_a\right)$. This also allows us to analyze the possible rank-1 connections among the variants of the low-symmetry configurations, concluding that there are not only (generic) conventional (type-1, -2, compound) twins, but also generic non-conventional (in hexagonal öptical" monoclinics and cubic monoclinics "cubic axes") non-generic (cubic monoclinics, both types and triclinics) and certain connections do not exist (in orthorhombics).Thus we fully classify the possibilities, providing formulars for the twin planes and the shear amplitude.

Precursor Oscillations

R.C. Rogers

I present a model of a solid-solid phase transitions that demonstrates a possible mechanism by which small amplitude oscillations in a symmetric austenite phase can be induced *before* a first order phase transition to finely twinned martensite. The model is one-dimensional and includes a triple-well potential with a central austenite well flanked by two martensite wells. The austenite well's height decreases with temperature as its concavity (elastic modulus at austenite) hardens. The first result I present shows that a combination of a soft austenite modulus and strong interaction with an internal variable or order parameter can cause a bifurcation to small amplitude oscillations *within* the austenite well. These branches of solutions would be either sub-critical or super-critical depending on the sign of the fourth derivative of the austenite well at its critical point. I also present a global bifurcation picture in the special case of multiple quadratic wells.

Recent Results on Extended Thermodynamics

T. Ruggeri

After a brief summary of the mathematical structure of the E. T. theory is presented, a state of the arts is given that includes

1. Equivalence of E. T. and the Maximum Entropy principle,
2. E. T. of high moments (wave velocities, light scattering, shock structure, wave velocities for increasing moments),
3. E. T. of radiation,
4. heat conductivity and bulk viscosity,
5. hydrodynamical models for semiconductors,
6. nesting theories.

In particular, it is shown that for a symmetric hyperbolic system with a convex extension it is possible to define principle subsystems that satisfy a subentropy law and subcharacteristic conditions hold. As a consequence, it is proven that the maximum characteristic velocity increases when the number of moments increases and tends to infinity in a classical theory while in the relativistic case the maximum is bounded by the speed of light.

Adaptive Optimization of Airfoils by Shape Memory Alloys

S. Seelecke

Airplanes of the future will have wings that adapt to changing flow conditions by optimizing their shape during the flight. This can be done by a grid of shape memory wires applied to the surface of the airfoil. Upon heating, the individual segments of the grid contract, and - within certain limits - one can obtain arbitrarily shaped profiles. Some optimal shapes are derived from the potential theory of aerodynamics, and a model for a shape memory wire is presented, which is capable of simulating the time evolution of the deformation when the wire is heated. Finally, as a first step to use it as a control device, the wire is coupled to an elastic beam, and the resulting bending problem is solved.

An Extended Moment Method in Radiative Transfer: The Matrices of Mean Absorption and Scattering Coefficients

H. Struchtrup

The goal of radiation thermodynamics is the determination of the transfer of radiative energy and momentum as well as of the interchange of energy and momentum between radiation and matter.

In principle the problem is solved when the radiative transfer equation with all interaction terms is known. Of interest are the thermodynamic quantities energy, momentum, energy and momentum interchange, entropy, etc... They may be calculated from the photon phase density or the intensity of radiation and the spectral absorption and scattering coefficients by integration over all photon frequencies and directions. The photon phase density follows as the solution of the radiative transfer equation which is - in general - not analytically solvable.

An alternative approach to the problem is the method of moments: One derives moment equations from the radiative transfer equation and obtains an infinite set of partial differential equations which may replace the radiative transfer equation. Since it makes no sense to deal with an infinite number of equations one has to restrict attention to a limited number of moments. The question is how many and which moments are needed for a satisfactory description of radiative processes.

Multiplication of the radiative transfer equation with $k^r n_{\langle i_1} \cdots n_{i_n \rangle}$ and subsequent integration over the wave-vector $k_i = k n_i$ yields a set of transfer equations

for the moments

$$u^r_{(i_1 \cdots i_n)} = \int k^r n_{(i_1} \cdots n_{i_n)} f \, d\mathbf{k},$$

where f is the photon distribution function.

The closure by means of the entropy maximum principle leads to a closed set field equations for the moments. The field equations are coupled by matrices of mean absorption and scattering coefficients.

We chose the moments $u^r_{(i_1 \cdots i_n)}$ with $r = 0, 1, \ldots, R$; $n = 0, 1, \ldots, N$ as variables and discuss which values R, N must be chosen in order to obtain reasonable results.

To do this we consider two simple processes, the homogeneous compression and relaxation of radiation and a beam which imerges into an atmospere. Both processes are calculated from the radiation transfer equation as well as from the moment equations. Comparision of the results leads to values for R and N.

Cahn-Hilliard Hydrodynamics

L. Truskinovsky

We develop a new "partial miscibility" regularization of the classical Navier-Stokes equations which provide a continuum description of the interface region between immiscible fluids. An additional scalar field is introduced to describe the concentration of one of the fluid components in a mixture. The resulting system of equations couples the fluid flow with a compressible version of the Cahn-Hilliard diffusion. An important feature of this model is the nonhydrostatic nature of the stress tensor even in the absence of viscosity, which gives rise to the effects of surface tension. We show that unless densities of the constituents are perfectly matched the straightforward incompressibility assumption has to be substituted by what we refer to as quasi-incompressibility (kinematic pressure enters the expression for the chemical potential). We establish some gereral properties of the Cahn-Hilliard-Navier-Stokes system an study analytically and numerically some simple examples of topological transitions like droplet annihilation and breaking of jets.

Dynamics of Point Defects in Nematic Liquid Crystals

E.G. Virga

The topological theory of defects assigns a charge to every point defect exhibited by nematic liquid crystals. Complex phenomena have been observed in capillary tubes involving the appearance and disappearance, along the axis of the tube, of periodic arrays of defects with alternating sign of charge. Here we move a step towards understanding these phenomena by considering a simple system, which would serve as an instructive example. We develop a mathematical model fit to describe the evolution in time of three defects. We write the differential

equations that rule this peculiar dynamical system: they show, in particular, how a defect is dragged in the wake of another with a velocity which depends on the distance between them.

High Moment Methods applied to Light Scattering, Plane Harmonic Waves and Shock Structures

Wolf Weiss

The macroscopic state of a gas may be described by the 13 fields mass density, velocity, temperature, pressure deviator and heat flux. These quantities are defined as moments of the distribution function. The Boltzmann equation implies a set of transfer equations for these moments. However, the system is not closed, but it can be closed by Grad's moment theory or by the maximization of the entropy.

There are circumstances where this system does not agree sufficient to the measurements.. In that case one can derive a system of equations for more than 13 moments. These high moment theories are applied in the following several phenomena.

- In a light scattering experiment a laser beam passes trough a gas and it is due to the microscopic fluctuations of the density that the laser light will be scattered. The spectrum of the scattered light is observed under the scattering angle θ, which is the angle between the laser beam and the photomultiplier. If θ is small then the large fluctuations are observed, while small fluctuations become detected for large θ.
- In an resonator the phase velocity and the damping of plane harmonic waves are measured as functions of the frequency.
- In a stationary one-dimensional shock one can observe the density profile for different Mach numbers.

For large values of scattering angle, frequency and Mach number many moments are needed to describe the process satisfactorily. Thus if in a given process the moments changes rapidly in space or time, or the process is far from equilibrium many moments are needed to describe such an process.

Thermodynamics of Multicomponent Porous Materials with the Balance Equation of Porosity

K. Wilmanski

The work is devoted to the construction of the thermodynamical model of the multicomponent porous material which is described by the following fields:

$\{\rho^S, \rho', \ldots, \rho^A\}$ partial mass densities of the skeleton and of the A fluid components, χ^S - motion of the sleleton, χ'^α - partial velocities of fluid components, n - porosity, θ - common temperature of components, all of them defined of the reference configuration of the skeleton $\mathcal{B}$ and time interval $\mathcal{J}$. It is assumed that the porosity n is driven by its own balance equation

$$\frac{\partial n}{\partial t} + Div\mathbf{J} = \hat{u}, \qquad \mathbf{J} - \text{ flux of porosity, } \hat{u} - \text{ source of porosity.}$$

This equation is motivated by the averaging of the changing geometry of the microstructure. Certain properties of static and kinematic interactions of components are discussed in details.

Thermomechanics of a Peptide Chain

H. Zorski

The considered peptide chain is assumed to be a smooth deforming line, each point having both translational and rotational degrees of freedom. There are the following kinematical constraints:

1. every cell is assumed to be a rigid body,
2. there are only two (dihedral angles) relative degrees of freedom beween adjacent cells.

The internal energy is invariant with respect to rigid motions and local; the appropriate expressions are proved to describe also the hydrogen bonds (non-local in the continuum). The whole system is described by 16 first order PDE's; it was derived by Zorski and Infeld. Now, the temperature is introduced and the final equations and the second law are derived following Liu's procedure. Appropriate kinematical assumptions e.g. the rotation axis is constant, lead to exact solutions. Thus, in the variable $\xi = s - Vt$, where s is a parameter along the continuous chain and V is a constant velocity, there is a following exact solution: the temperature is a classical kink (hyperbolic tangent) and the line, starting from $\xi = -\infty$ is a helix (almost) as long as the temperature is constant (almost), than it breaks away. From the cylinder, and when the temperature becomes again constant, the curve again approaches a helix wound around a different cylinder. This solution may be regarded as an elementary act of destruction and healing of the helix by a temperature kink. It may play part in solving the problem of folding of peptide chains.

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