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This workshop on the interaction of modern mathematical methods in nonlinear partial differential equations and applications in materials science was organized by J.M. Ball (Mathematics, Oxford), R.D. James (Mechanical and Aerospace Engineering, University of Minnesota) and S. Müller (MPI for Mathematics in the Sciences). It covered a broad range of applications ranging from Bose-Einstein condensates to thin magnetic and elastic films, biomaterials, geological materials and materials undergoing solid-solid phase transformation. These rather different applications areas are connected by a clear common theme, both from the point of view of mathematical analysis and from the point of view of applications. In almost all of the problems discussed it crucial is to analyse and bridge the many different scales which are present. In the last years a number of new mathematical tools have been developed to address this problem and the workshop gave an impressive overview of the achievements as well as the challenges ahead. Of particular value, both for the experts and the many younger participants was the opportunity to contrast the new mathematical ideas with experimental findings and challenges. The intense atmosphere at Oberwolfach and the excellent library provided a perfect framework for such an exchange.

The organizers and the director at Oberwolfach, G.-M. Greuel (Kaiserslautern), are pleased to thank the European Science Foundation for supporting this workshop as an Exploratory Workshop (EW 02-83). In particular, this concerns the participation of 20 younger mathematicians from Europe in the workshop.

Programme

(In the order of the talks.)

- F. Otto: Excitations in thin film ferromagnetic elements
- S. Bianchini: Asymptotic Behavior of Smooth Solutions for Dissipative Hyperbolic Systems with a Convex Entropy
- A. Aftalion: Mathematical model for Bose Einstein Condensates
- A. DeSimone: Modelling granular materials with crushable grains
- A. Schlömerkemper: Discrete-to-continuum limit of a magnetic force
- X. Blanc: Crystalline symmetry and energy minimization
- M. Ortiz: Variational Methods in Dislocation Dynamics
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- R. Schätzle: Solutions of the Stefan problem with Gibbs-Thomson law without global minimization

Abstracts

Excitations in thin film ferromagnetic elements

F. OTTO

Motivation for this joint work with Ruben Cantero-Alvarez is the following experimental observation for thin film ferromagnetic elements. Elements with elongated rectangular cross-section are saturated along the longer axis by a strong external field. Then the external field is slowly reduced. At a certain field strength, the uniform magnetization switches into a quasiperiodic domain pattern which resembles a concertina (Akkordeon).

Starting point is the 3-d micromagnetic model (energy functional E with exchange and stray field energy). To simplify the analysis, we consider a thin-film element of infinite length (in x_1), width ℓ (in x_2) and thickness t (in x_3). For this geometry, the uniform magnetization $m^* = (1, 0, 0)$ is a stationary point for any external field $(H_{ext}, 0, 0)$. We investigate the Hessian $\text{Hess}E(m^*)$. What is the strength H_{ext}^* of the external field at which the m^* becomes unstable, i. e. $\text{Hess}E(m^*)$ no longer positive definite? We rigorously identify exactly four different regimes with different scaling laws for H_{ext}^* in the parameters ℓ , t , d (exchange length).

The largest of these regimes has modes (= eigenfunctions of $\text{Hess}E(m^*)$ corresponding to the zero eigenvalue at H_{ext}^*) which have a periodic structure in x_1 -direction of period

$$w = \left(32\pi \frac{\ell^2 d^2}{t} \right)^{1/3}.$$

This can be seen by identifying the Γ -limit of the Rayleigh coefficient for the Hessian (no external field) w. r. t. the L^2 -inner product.

For a wide range of widths ℓ and thicknesses t (factors of eight), this theoretical w agrees well (factors of 1 to 2) with the experimentally observed period of the concertina pattern. This leads us to conjecture that the length scale of the concertina pattern is the frozen-in length scale of the most unstable excitation of the uniform magnetization.

Asymptotic Behavior of Smooth Solutions for Dissipative Hyperbolic Systems with a Convex Entropy

S. BIANCHINI

(joint work with B. Hanouzet)

We establish a result of stability for small perturbations of constant equilibrium states for general entropy dissipative hyperbolic systems, under the Kawashima condition. We show that global smooth solutions approach the constant state in the L^2 -norm at a rate $O(1+t)^{-1/4}$, as $t \rightarrow \infty$. The result extends the previous one by Denis Serre, who assumed zero mass for the initial perturbation. The proof is based on a refined analysis of the Green function for the linearized problem, which is decomposed in three main terms. The first one, which takes into account for the diffusive effects, is shown to vanish when applied to the source term. The second one decays at an exponential rate. Finally the remainder term decays faster than the diffusive one. This analysis improves on previous results, and

in particular no assumptions are made on the symmetry properties of the jacobian of the source term.

Mathematical model for Bose Einstein Condensates

A. AFTALION

One of the key issues related to superfluidity is the existence of quantized vortices. Following recent experiments on Bose-Einstein condensates exhibiting vortices, we investigate the behavior of the wave function which solves the Gross Pitaevskii equation. For a rotating Bose-Einstein condensate in a harmonic trap, we give a simplified expression of the Gross-Pitaevskii energy in the Thomas Fermi regime, which only depends on the number and shape of the vortex lines. This allows us to study in detail the structure of the line of a single quantized vortex, which has a U or S shape. S type vortices exist for all values of the angular velocity Ω but are not minimizers of the energy while U vortices are minimizers and exist only for Ω sufficiently large. We also show 3d simulations of solutions.

Modelling granular materials with crushable grains

A. DESIMONE

Granular materials with crushable grains exhibit a complex mechanical response due to changes of their internal structure induced by the application of loads. Interest in their behavior is related to problems in geotechnical engineering, powder compaction, and in the food and pharmaceutical industry. Moreover, since much of their response is controlled by the evolution of the underlying granular structure, these materials offer an opportunity to assess critically classical constitutive models of granular matter based on a continuum description.

In this work, a procedure to deduce a strain-hardening elastoplastic model from an experimentally measured stress-dilatancy curve is described. The procedure requires the existence of a one-to-one stress-dilatancy relation, as it is experimentally observed for a wide class of granular materials with permanent grains. To cope with the case of crushable grains, an internal variable M is introduced, which describes the intrinsic frictional properties of a granular assembly, and which evolves as grain crushing proceeds. The stress-dilatancy behavior is now described by a one-parameter family of curves, parametrized by M . This delivers a new constitutive model which is able to reproduce the observed response of a weak pyroclastic rock exhibiting grain crushing.

The evolution of M , which physically corresponds to the evolution of the grain size distribution, is responsible for a softening mechanism which promotes the formation of shear bands. This is associated with the loss of convexity of the variational problem defining the incremental response of the material.

This is joint work with M. Cecconi, C. Tamagnini, and G.M.B. Viggiani.

Discrete-to-continuum limit of a magnetic force

A. SCHLÖMERKEMPER

We discuss a mathematically rigorous derivation of a formula for the magnetic force between two parts of a magnetic continuous body.

On a Bravais lattice of magnetic dipoles the force between the dipoles in a part of a bounded subset of \mathbf{R}^3 and its complement is considered. For the passage to the continuum an appropriate force formula is formulated on a scaled lattice and the continuum limit is performed by letting the scaling parameter tend to zero. This involves a regularization of the occurring hypersingular kernel and a suitable reorganization of a lattice sum in the spirit of that by Cauchy in elasticity theory.

It turns out that the limiting formula is different from a corresponding force formula which has been known for long in the literature (cf. e.g. W. F. Brown). The limiting force formula shows a dependence on the structure of the underlying lattice.

Crystalline symmetry and energy minimization

X. BLANC

The subject of the talk is the understanding of the emergence of crystalline order at low temperature. Mathematically speaking, we state the problem as follows: consider a set of N identical atoms in their ground state. Is this configuration periodic, or does it become periodic as N goes to infinity? We will expose results on quantum models in dimension one, and numerical evidence in dimension two for two-body models.

Variational Methods in Dislocation Dynamics

M. ORTIZ

A phase-field theory of dislocation dynamics, strain hardening and hysteresis in ductile single crystals is developed. The theory accounts for: an arbitrary number and arrangement of dislocation lines over a slip plane; the long-range elastic interactions between dislocation lines; the core structure of the dislocations resulting from a piecewise quadratic Peierls potential; the interaction between the dislocations and an applied resolved shear stress field; and the irreversible interactions with short-range obstacles and lattice friction, resulting in hardening, path dependency and hysteresis. A chief advantage of the present theory is that it is analytically tractable, in the sense that the complexity of the calculations may be reduced, with the aid of closed form analytical solutions, to the determination of the value of the phase field at point-obstacle sites. In particular, no numerical grid is required in calculations. The phase-field representation enables complex geometrical and topological transitions in the dislocation ensemble, including dislocation loop nucleation, bow-out, pinching, and the formation of Orowan loops. The theory also permits the consideration of obstacles of varying strengths and dislocation line-energy anisotropy. The theory predicts a range of behaviors which are in qualitative agreement with observation, including: hardening and dislocation multiplication in single slip under monotonic loading; the Bauschinger effect under reverse loading; the fading memory effect, whereby reverse yielding gradually eliminates the influence of previous loading; the evolution of the dislocation density under cycling loading, leading to characteristic ‘butterfly’ curves; and others.

Mathematical and Numerical Analysis of micromacro models for polymeric fluids

C. LEBRIS

The so-called micromacro models for polymeric fluids consist in coupling the macroscopic conservation equations with a microscopic kinetic equation describing the evolution of the polymeric chains. The motivation is to bypass the writing of a constitutive law, which is most often ignored. From the mathematical standpoint, the difficulty lies in the coupling of a partial differential equation with a stochastic partial differential equation. Existence and uniqueness results for the Cauchy problem can be proven, as well as a complete numerical analysis for a simplified case, namely the Couette flow. The approach and the techniques can be applied to slightly different contexts: that of the modelling of muds and suspensions, and that of the modelling of elastomers. All this is joint work with B. JOURDAIN, T. LELIEVRE, E. CANCÈS, Y. GATI (Ecole des Ponts), I. CATTO (Paris 9), and P.L. LIONS (Collège de France).

Statistical Mechanics and Nonlinear Elasticity

O. PENROSE

A scheme is proposed for defining the free energy per particle in a molecular model of a solid, as a function of the elastic deformation matrix (the “stored energy function” of nonlinear elasticity theory). The free energy is defined as usual by $F = -kT \log Z$, where $Z = \text{const.} \int e^{-H/kT}$ and H is the Hamiltonian of the microscopic particle system, T is the temperature and k Boltzmann’s constant, but here the integration is restricted to configurations satisfying a “tiling condition” which requires the local configuration near every particle to lie within a specified standard set of configurations. As an illustration, the method is applied to a simple two-dimensional model in which twinning is possible; for this model it is possible to show that the thermodynamic limit of the free energy per particle exists, is independent of the shape of the container, and is a continuous quasi-convex function of the deformation matrix.

Finite elasticity of curved lattices: application to carbon nanotubes

MARINO ARROYO

(joint work with T. Belytschko, Northwestern University)

A method for the passage from lattice models to continuum mechanics models for lattice systems of reduced dimensionality is presented. The traditional methods of finite crystal elasticity, valid for space-filling crystals, are extended to deal with crystalline monolayers in 3D. First, it is postulated that the continuum object is also of reduced dimensionality, i.e. a surface. Then, motivated by the geometry of the deformation of such objects, an extension of the Cauchy-Born rule is proposed. This kinematic assumption relates the deformation of the continuum to that of the discrete system, and allows us to formulate hyper-elastic constitutive relations based exclusively on the underlying lattice model. This model is applied to carbon nanotubes, and by comparing numerical calculations of the continuum model discretized with finite elements with atomistic calculations, it is found that the surface model very accurately mimics the parent discrete model in the full nonlinear

regime. The finite element discretized version of the model provides a computationally advantageous alternative to full atomistic calculations.

Modeling of frictionless contacts and self-contacts for deformable bodies

O. PANTZ

We proposed a new modeling of frictionless (self-)contacts for deformable bodies, available for thin structures as well as for genuine bodies. For simplicity, we consider elastic bodies. In a classical way, the equilibrium state is described as the minimizer of the energy on a set of admissible deformations. The main challenge here is to define a good set of admissible deformations, that is such that:

- If the initial minimization problem (without the constraint of non-self intersection) is well posed, it remains well posed for the constrained one.
- A minimizer (at least regular) of the energy must fulfill the Euler-Lagrange equations.

Our modeling respects both of those points in most cases. However, in the case of shells, the second point is not always respected. Finally, our modeling leads to a new algorithm based on the introduction of a penalization function.

Rank-one convexity and Nonlinear elliptic systems

L. SZEKELYHIDI

We addressed the question of what are appropriate assumptions on the ellipticity in quasilinear systems to ensure a good regularity theory. Our work was motivated by the example constructed by S. Müller and V. Šverák in '99 of a strongly quasiconvex functional admitting Lipschitzian critical points which are nowhere C^1 (this should be compared to the result of L. C. Evans saying that minimizers of such functionals are partially regular). We presented an extension of this work to polyconvex functionals. This method relies on being able to show that the rank-one convex hull of a certain four-dimensional manifold in the space of 4×2 -matrices related to the PDE can be large, and in this quest certain finite-point configurations of matrices (T_N -configurations) play a decisive role.

A justification of the nonlinear Kirchhoff-Love model of plates, using a new singular inverse method

R. MONNEAU

In the framework of isotropic homogeneous nonlinear elasticity for a St. Venant-Kirchhoff material, we consider a three-dimensional plate of thickness ε and periodic in the two other directions. Using a new method that we call the *Singular Inverse Method*, we prove the existence of a rescaled solution uniformly in ε for small forces, and at the same time, we prove the rigorous convergence of this rescaled solution to the solution of the nonlinear Kirchhoff-Love plate model. We also state a 3d-2d error estimate.

Mathematical analysis of long-range interatomic forces arising from quantum mechanics

G. FRIESECKE

According to quantum mechanics, atoms interact directly through a field equation containing the atomic positions as parameters (the many-electron Schrödinger equation). We show rigorously that e.g. for two hydrogen atoms, the ground state energy of the system minus the energy of the individual atoms behaves like $-\frac{c_6}{r^6}$ as $r = \text{interatomic distance} \rightarrow \infty$ (van der Waals interaction), and give a formula for c_6 . Trial functions giving an upper bound with correct scalings are well known in the physics literature, but the lower bound is new and the correct formula for c_6 disagrees with an accepted expression. As a corollary we are able to decide whether or not the N -atom interatomic potential decomposes at long range into a sum of pair potentials. (Yes for hydrogen; answer conjectured to depend on type of atom in a simple way.)

Some aspects of myocardium modelling

A. RAOULT

The myocardium is a thick muscle whose fibre organization cannot be understood by means of classical dissection techniques. Streeter conjectured in 1979 that myocardium fibres were organized as closed geodesics running on a set of toroidal surfaces. Recent measurements obtained by means of quantitative polarized light microscopy made it possible to determine the fibre direction in a large part of the ventricles. The Clairaut property, which is valid for surfaces of revolution, states that the product $r \cos \theta$, where for any point M , r denotes the distance to the axis of revolution and θ is the angle at point M between the curve and the parallel remains constant along a geodesic. Using the experimental data provided to us, we were able to check in the case of the left ventricle several consequences of the Clairaut property, such as the fact that the traces on horizontal sections of the isovalues of the Clairaut number actually are two concentric circles.

The full understanding of the claimed geodesic nature of the fibres requires a mechanical modelling of the myocardium and the determination of an optimization criterion. We first concentrate on the derivation of a nonlinear constitutive law. Noticing that fibres and the overall muscle gain their contractile properties from the myocytes, we choose to use a discrete homogenization technique where myocytes behave as bars between nodes – that represent the anastomoses – and where myocytes interact by moments. The length at rest introduced as a parameter is a first step towards taking into account the electrical activation. The resulting constitutive law of the equivalent continuous medium is obtained by solving a self-equilibrium system on a reference brick of the lattice. Comparisons with existing laws for soft tissues are made by means of numerical simulations of elementary deformations.

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Asymptotics of the Becker-Döring equations

B. NIETHAMMER

(joint work with P. E. Jabin)

We consider the long-time behaviour of solutions to the Becker-Döring cluster equations. It is well known that if the total density of atoms exceeds a critical value, the excess density is contained in larger and larger clusters as time proceeds. We rigorously derive that the dynamics of the large clusters are described by a non-local transport equation. The proof exploits the energy-energy dissipation relation given by the Lyapunov functional for the Becker-Döring equations.

We also use the energy estimate to derive an explicit rate of convergence to equilibrium in the case of subcritical density. Due to the structure of the equilibrium no logarithmic Sobolev inequality is available. We show a weaker inequality which implies for fast decaying data a convergence rate of the form $e^{-c_0 t^{1/3}}$.

Twin boundaries: superhighways or parking lanes

E. SALJE

Twin boundaries are shown to enhance or reduce the mobility of dopants. Typical examples are ferroelastic WO_3 (with fast Na transport) and PbTiO_3 for oxygen vacancies. Coupled order parameter models are shown to be good model in the continuum limit. ‘Atomistic’ discrete models are applied for such cases together with surface relaxations. It was shown that reduced transport along $[0,0,1]$ in α -quartz is due to a specific internal structure inside the twin boundary which reduces the diameter of the structural bottle neck for Li and Na. Dynamical movements of boundaries are dominated by retracting needle domains rather than sid-way movements.

Finite-Strain Elasto-Plasticity

A. MIELKE

The classical flow-law formulation of rate-independent, finite-strain elastoplasticity is replaced by a purely energetic formulation which is based on the storage functional \mathcal{E} and the dissipation distance \mathcal{D} . Sufficiently regular solutions of this formulation also solve the flow-law formulation. However, the energetic formulation is derivative-free and it motivates the time-incremental problem

$$(IP) \quad (\varphi_k, P_k, p_k) \in \operatorname{argmin} \mathcal{E}(t_k, \varphi, P, p) + \mathcal{D}((P_{k-1}, p_{k-1}), (P, p))$$

which can be approached by methods from the nonconvex calculus of variations. Existence results for (IP) are presented for $d = 1$ and $d = 2$.

Brittle Fracture Evolution in a Quasi-static Setting

G. A. FRANCFORT

This work results from various collaborations with B. BOURDIN, G. DAL MASO, C. LARSEN, J.J. MARIGO and R. TOADER.

We propose a variational model for quasi-static brittle fracture. From a mechanical standpoint, the model is very close in spirit to that of Griffith (around 1920). It consists

in minimizing at each time the sum of the elastic and surface energies (proportional to the crack surface area), subject to:

1/irreversibility: the crack never heals;

2/energy balance: the total derivative of the energy balances the power of the external loads.

From a mathematical standpoint, we start with a sequence of time discretized problems in $SBV(\Omega)$, the jump part of the test fields corresponding to the add-crack at a given time. We then pass to the limit in the time discretization, thanks to a geometric measure theoretic result, which roughly states that, if $u_n \rightharpoonup u$, weakly in $SBV(\Omega)$ with ∇u_n bounded in $L^p(\Omega)$, $p > 1$, then, for any $v \in SBV(\Omega)$ such that $S(v) \subset S(u)$, we can find $v_n \in SBV(\Omega)$ such that $v_n \rightarrow v$ in $L^1(\Omega)$, $\nabla v_n \rightarrow \nabla v$ in $L^p(\Omega)$, and $\limsup \mathcal{H}^{N-1}(S(v_n) \setminus S(u_n)) \rightarrow 0$.

We ultimately show existence for the proposed model.

Finally, we illustrate our model with various computations, which seem to qualitatively agree with experimental results.

On some problems related to crack propagation

G. OLEAGA

In this work we approach the problem of finding a relationship between the direction of crack propagation in a brittle solid and the elastic field surrounding the tip avoiding unessential physical assumptions. We apply basic principles of mechanics such as *Fourier's inequality* in the case of quasistatic propagation and an incremental version of *Hamilton's principle* for the dynamic case (i.e. including forces of inertia). By means of adequate *inner variations* of the field we obtain a balance of non classical forces similar to the one obtained by other authors. This balance holds only for smooth crack paths and when expressed in terms of the *stress intensity factors* yields the well known *principle of local symmetry* proposed previously for quasistatic propagation and extensively applied in the computation of stability of crack paths and crack front waves in the dynamical case.

Derivation of nonlinear rod theories from 3D nonlinear elasticity by Γ -convergence

M. G. MORA

A fundamental problem in nonlinear elasticity is to understand the relation between three dimensional theory and lower dimensional theories for thin domains.

In this talk (which is on joint work with Stefan Müller) we rigorously deduce some nonlinear models for rods passing to the limit in the functional of the elastic energy $E^{(h)}$ as the diameter h of the rod goes to zero. The limit is taken in the sense of Γ -convergence.

What distinguishes the different models, is the order of magnitude of $E^{(h)}$ in terms of h . Scaling the energy $E^{(h)}$ by h^4 we derive a model for inextensible rods where the admissible deformations are bending flexures and torsions keeping the middle fiber unstretched.

As $E^{(h)}$ is of the order of h^6 , the corresponding deformations are close to a rigid motion, so that one can linearize around it and obtain at the limit a theory analogous to the Föppl-von Kármán theory for plates.

On the modelling of cooling lava by nonlinear elasticity

M. JUNGEN

(joint work with J. M. Ball)

We discuss a model in which nonlinear elasticity theory is used to describe the formation of cracks in elastic bodies subject to thermal stresses. In particular, we are trying to understand the enigmatic fracture process in cooling lava which gives rise to the formation of column joints. Column joints consist of basalt columns which are characterised by their polygonal cross-section and usually feature a strikingly high degree of regularity. Although several attempts were made to understand how the cooling process can lead to such features, none of the proposed models so far are entirely satisfactory from a physical point of view. The presented work is based on the idea that columnar jointing could be well understood and described with an appropriate model based on nonlinear elasticity.

Can we fill the gap between quasiconvexity and polyconvexity with elliptic PDEs?

D. FARACO

In this talk we present examples of non-polyconvex quasiconvex functions built on some partial differential equations. In particular we concentrate in Hessian equations and Beltrami equations.

For a symmetric matrix $A \in \mathbf{S}^{n \times n}$ the k -Hessian operator is defined by,

$$[A]_k = S_k(\lambda(A)),$$

where $\lambda(A)$ stands for the vector of eigenvalues of A and S_k is the k elementary symmetric function. The cone $\Gamma_k = \{A : [A]_j \geq 0 \text{ for } j = 1, 2, \dots, k\}$ can be thought of as the domain of ellipticity of the k -Hessian operator. The k -Hessian equations have been intensively studied recently by Trudinger and Wang, based on previous work of Caffarelli, Nirenberg and Spruck. Using this theory we proved the following theorem.

Theorem 1: (F., X. Zhong; ARMA 2003)

Let G_k be defined as

$$G_k(A) = \begin{cases} [A]_k & \text{if } A \in \Gamma_k, \\ 0 & \text{otherwise.} \end{cases}$$

Then G_k is quasiconvex on symmetric matrices.

The second part of the talk uses the invertibility of Beltrami Operators proved by Astala Iwaniec and Saksman to solve some questions posed by Kewei Zhang. The result is as follows.

Theorem 2: (F.; To appear in MM)

Let $E \in \mathbf{M}^{2 \times 2}$ s.t. $\forall A, B \in E : K \det(A - B) \geq |A - B|^2$.

a) Then if $p > \frac{2K}{K+1}$, $\exists C(p, K)$ s.t.

$$Q \text{ dist}_E^p \leq C(p, K) \text{ dist}_E^p.$$

b) $Q^p E = E$, if $\det(A - B) > 0$ and $\lim_{M \rightarrow 0} \sup_{A \in E \setminus B(0, M)} \frac{|A|^2}{\det A} \leq K$

c) $\exists E$ fullfilling the condition such that for $p < \frac{2K}{K+1}$

$$Q^p E = C(E).$$

The examples in E are of two kinds. Either we exhibit very weak solutions to an appropriate Beltrami equation or we construct suitable laminates. The method of convex integration seems to give a two ways correspondence between sets without rank-one connections with non-trivial p -quasiconvex hull and very weak solutions that we will investigate in the future.

Kinetics of martensitic phase transformations

K. BHATTACHARYA

This talk discusses free boundary problems in heterogeneous media and their homogenization motivated by the study of crystalline solids that undergo the martensitic phase transformation. This is a class of solid-to-solid phase transformations observed in crystalline solids. They are characterized by a discontinuous change of crystal structure with changing temperature and the lack of any rearrangement of atoms. Materials that undergo such transformations are observed to display fine scale microstructure: a complex arrangements of the different phases. The microstructure changes with applied load or changing temperature, and our interest lies in understanding the dynamics that govern the evolution of this microstructure.

These solids have long been modeled using a continuum theory. However, the classical equations of continuum physics are insufficient to describe the evolution. This information is often supplied from outside the theory in the form of a kinetic relation. This talk discusses how this kinetic relation may be obtained from microscopic considerations.

We begin by constructing a discrete model: a chain of atoms connected by bistable springs. We present numerical evidence that the dynamics of such chains are characterized by ‘travelling-wave type solutions’. We also present numerical evidence that these travelling wave type solutions induce a continuum kinetic relation.

We then turn to the influence of defects, and how they pin the interface. We present a continuum model which leads to a free boundary problem with rapidly varying coefficients. We discuss the homogenization of such a model, and its implication on the macroscopic kinetic relation.

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Elastic rods, Elastic Birods & the Mechanics of DNA

J. H. MADDOCKS

The sequent dependent mechanical properties of DNA at the length scales of 100-200 bp are generally believed to be central to the biological function and packing of DNA. I argue that given a basic base pair energy, it is efficient to pass to the continuum limit and perform analysis and computation in the elastic rod model. I then describe how to extract rigid-base pair models from Molecular Dynamics (MD) simulations of the atomistic system. These computations suggest that a rigid base model is directly superior to the rigid base-pair description. Passing to the continuum limit in the rigid base model yields a new continuum object that we call a birod. It can be viewed as a mixture theory for a rod model of each of the backbones of the DNA. It takes the mathematical form of a standard Cosserat rod endowed with an additional internal microstructure.

Solutions of the Stefan problem with Gibbs-Thomson law without global minimization

R. SCHÄTZLE

Global solutions of the Stefan problem with Gibbs Thomson law were obtained by Luckhaus in [1] using a global minimization process. As this global minimization is difficult to be justified from the thermodynamical point of view, M. Röger constructed in his doctoral thesis [2] new solutions of the Stefan problem with Gibbs Thomson law without global minimization.

The difficulty is that in the limit procedure area of the free boundary can be lost, and the Gibbs Thomson law is verified first in the measure theoretic sense using [3] and then determining the mean curvature on the phase separating parts of the free boundary in terms of approximate differentials of the height functions by an identity established in [4].

Keywords: Stefan problem, free boundaries, geometric measure theory, fully non-linear elliptic equations.

AMS Subject Classification: 35 R 35, 49 Q 15, 35 J 60.

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