On some multi-phase problems in continuum mechanics

Fluid mixtures—Fatigue—Strained semiconductors

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Aims

Modelling multi-phase systems and studying their asymptotic behaviour through the theory of dynamical systems

- binary fluids
- strained semiconductors
- fatigue in polycrystalline metals
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- binary fluids
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Contents

1. Asymptotic behaviour of fluid mixtures
2. Strain in semiconductors
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1. Asymptotic behaviour of fluid mixtures

2. Strain in semiconductors
Main problem

Modelling questions:
- How can quenching of metals be characterised?
- What can diffuse interface models tell on polymer mixtures?
- How can the insurgent patterns be described?
- Do nonlocal interactions play a significant role?

Mathematical issues:
- Navier-Stokes equations \(\rightarrow\) well-posedness problems in 3D
- physically significant singular potential
- separation property
- regularity theory
Modelling phase separation

Free energy:
\[
\Phi = \frac{\epsilon}{2} \int |\nabla \psi|^2 + \frac{1}{\epsilon} \int f(\psi)
\]

surface tension \quad double well

A gradient flow approach gives
\[
\alpha \partial_t \psi = \Delta(-\epsilon \Delta \psi + \frac{1}{\epsilon} f(\psi))
\]

\(\alpha\): relaxation parameter
\(\sqrt{\epsilon}\): interaction length
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\( f(\psi) \)

homogeneous phase
Modelling phase separation

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cooling
Modelling phase separation

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surface tension → double well

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fluctuations $\rightarrow$ phase separation
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\( \Phi \): NOT a phase transition!
The Cahn-Hilliard equation I

\[ \begin{cases} \partial_t \psi + (\mathbf{v}(t) \cdot \nabla)\psi = \Delta (f'(\psi) - \Delta \psi) \\ \partial_{\nu}\psi = \partial_{\nu}\mu = 0 \end{cases} \]

No mass flux; phase interfaces “orthogonal” to boundary

Mass conservation

\[ \int_{\Omega} \psi(t) = C \]
The Cahn-Hilliard equation I

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Mass conservation

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The Cahn-Hilliard equation II

Thermodynamically significant singular potential:

\[ f(\psi) = (1 + \psi) \log(1 + \psi) + (1 - \psi) \log(1 - \psi) \]

\[ + (1 - \psi)(1 + \psi) + C \]

This potential is often regularised by taking

\[ f(\psi) = |\psi|^{2l} - \psi^2 \]

\[ l \in \mathbb{N}, l \geq 2 \]
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convex part

\[ + (1 - \psi)(1 + \psi) + C \]

Lip. part

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On nonlocal interactions

Nonlocal interacts between particles of the mixture

Kac potentials: \( \gamma^n K(\gamma |x - y|), \quad \gamma > 0 \)

A hydrodynamic limit leads to the total energy

\[
E_P(\psi) \propto \int\int_{\Omega \times \Omega} K(|x - y|)|\psi(x) - \psi(y)|^2 + O.T.
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Regular kernel \( K \in W^{1,1} \)
- second-order integro-differential equation
- studied by Frigeri, Grasselli et al.

Singular kernel \( K(y) \propto |y|^{-n-\alpha} \)
- formal structure of CH equation preserved
- incomplete regularity theory
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The Cahn-Hilliard-Navier-Stokes system

\[ \Omega \in \mathbb{R}^n, \; n = 2, 3 \]

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\begin{cases}
\partial_t u + (u \cdot \nabla)u = -\nabla p + \nabla \cdot (\tau(\nabla u)) - \nabla \cdot (\nabla \psi \otimes \nabla \psi) + g(t) \\
\nabla \cdot u = 0 \\
\partial_t \psi + (u \cdot \nabla)\psi = \Delta \mu \\
\mu = \frac{1}{\epsilon} f'(\psi) - \epsilon \Delta \psi
\end{cases}
\]

Main assumptions

- stress-deformation rate relation
- chemical potential
- diffusion operator

\[ f'(\psi) = \begin{cases} 
\psi^3 - C_\theta \psi \\
- C_\theta \psi + \log \frac{1+\psi}{1-\psi}
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Some background

The model H has been widely studied

- 2D, \( \exists! \) (Starovoitov '97, Boyer '01) long-time behaviour (Wu et al. '09, Gal and Grasselli '10)
- Singular potential: \( \exists! \), global attractor, convergence to stationary states (Abels '09)
- nonlocal (smooth kernel) with regular and singular potential: \( \exists! \), large-time behaviour (Frigeri, Grasselli et al. '12)

The nonlocal CH model was rigourously derived by Giacomin and Lebowitz (1996)
Infinite dimensional dynamical systems—attractors

Main tools:
- global attractor
- trajectory attractor
- exponential attractor
- pullback attractor

Basic issues:
- compactness
- finite-dimensionality
- invariance
- rate of attraction

This point of view is complementary to the study of convergence to stationary states
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Semigroups

Definition

A family \( \{S(t)\}_{t \geq 0} \), \( S(t) : X \to X \) is a \textit{semigroup} on \( X \) if

- \( S(0) = I \)
- \( S(t)S(s) = S(t + s) \) for any \( s, t \geq 0 \)

Definition

A set \( B \subset X \) is \textit{absorbing} for \( \{S(t)\}_{t \geq 0} \) if for any bdd set \( B \subset X \) there exists a time \( t_B \geq 0 \) s.t. \( S(t)B \subset B \) for all \( t \geq t_B \)
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Global attractors

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A set $\mathcal{A} \subset X$ is the global attractor for $\{S(t)\}_{t \geq 0}$ if it is
- compact
- invariant
- minimal
- attracting

Theorem
If $\{S(t)\}_{t \geq 0}$ possesses a compact absorbing set then it has a global attractor

If it exists, the global attractor is unique
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Exponential attractors

**Definition**

A compact and finite-dimensional set, which attracts all bdd sets of initial data exponentially fast, is called *exponential attractor*

Exponential attractors may not be unique

**Definition**

Let $X_1 \subseteq X$, then $\{S(t)\}_{t \geq 0}$ has the *smoothing property* if there exist $t \geq 0$, $C$ and a bdd absorbing set $B \subset X$ s.t.

$$\forall x, y \in B, \quad \|S(t)x - S(t)y\|_{X_1} \leq C\|x - y\|_X$$

**Theorem**

If $\{S(t)\}_{t \geq 0}$ has a bdd absorbing set on which the smoothing property holds at time $t_0$, then the discrete semigroup $\{S(kt_0)\}_{k \in \mathbb{N}}$ has a *discrete-time exponential attractor*
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Our results

4 different settings

- non-newtonian fluids (shear thickening, Ladyzhenskaya type)
  3D, singular potential
  $\rightarrow$ existence, trajectory attractor

- chemically reacting fluids, 2D regular potential
  $\rightarrow$ well-posedness, robust family of exponential attractors

- original system, potential with arbitrary polynomial growth
  $\rightarrow$ pullback exponential attractor

- nonlocal diffusion
  $\rightarrow$ existence, regularity
Non-newtonian fluids


Shear-thickening fluid

$$\tau(\nabla u) : \nabla u \geq C_N |\nabla u|^2 + C_L |\nabla u|^p$$

This gives the energy identity also in the 3D case
Uniqueness is open (singular potential) in contrast to the
uncoupled equations

Assumptions
- singular potential
- order-parameter-dependent viscosity
- non autonomous forcing term

Results
- existence
- global long-time behaviour (trajectory attractor in weak and strong topologies)
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Polymer models - Chemically reacting fluids


We consider chemical reaction between the two phases (e.g. transition between two polymer configurations) \( \rightarrow \) changes to pattern formation

\[
\partial_t \psi + (u \cdot \nabla) \psi + \delta(\psi - c_0) = \Delta \mu
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Results (2D, regular potential)
- existence and uniqueness
- global long-time behaviour (robust exponential attractor)

Open problems and ongoing work
- convergence to stationary states?
- pullback (exponential) attractor
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Exponential pullback attractors

Bosia, Gatti - submitted

The pullback attracting property can be written as

$$\lim_{t \to -\infty} d(U(s, t)z, A(s)) = 0$$

The attractor is the set of possible current configurations for a system that has been evolving for a (infinitely) long time.

Assumptions (2D)

- regular potential (arbitrary fast polynomial growth)
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Results

- existence
- regularity estimates depending on the growth of the potential only through constants
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Nonlocal interactions

Abels, Bosia, Grasselli - submitted

The chemical potential is given by

\[(\mu, \varphi) = \mathcal{E}(\psi, \varphi) + (f'(\psi), \varphi) \quad \forall \varphi \in H^{\alpha/2}\]

\(\mathcal{E}\) is the “regional fractional laplacian”

\[\mathcal{E}(u, v) = \iint_{\Omega \times \Omega} K(x - y)(u(x) - u(y))(v(x) - v(y))\]

Results (CH , 3D, singular potential)

- well-posedness (variational)
- regularity results (continuity)
- characterisation of boundary conditions for regular solutions
- global attractor

Open problems

- regularity up to the boundary
- notion of solution
- convergence to stationary states
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Theorem

Let $\psi_0 \in H^{\alpha/2}$, $\Phi(\psi_0) < \infty$ then there exists a unique weak solution s.t.

$$
\psi \in C(H^{\alpha/2}_0) \quad \partial_t \psi \in L^2(H_0^{-1}) \quad \mu \in L^2(H^1)
$$

Moreover there hold

$$
\Phi(\psi(t)) + \int_0^t |\nabla \mu| = \Phi(\psi_0) \quad \forall t > 0
$$

if $n \leq 3$ \quad $\psi \in L^\infty(C^\beta)$ \quad for some $\beta > 0$

and the associated semigroup has a (connected) global attractor

WARNING! The expected $L^2(H^\alpha)$ regularity is unknown
Nonlocal interactions II
Existence and uniqueness

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A sketch of proof

Let $\mathcal{E}(\psi, \varphi) = (\mathcal{L}\psi, \varphi)$, $\forall \psi, \varphi \in H^{\alpha/2}$

- well posedness of the problem (compactness and monotonicity arguments)

$(\mu, \varphi) = \theta(\nabla \psi, \nabla \varphi) + \mathcal{E}(\psi, \varphi) + (f'(\psi), \varphi)$

- limit $\theta \to 0$

- attractor: a compact absorbing set is given by

$\mu - f'(\psi) \in L^2 \subset H^{-\alpha/2}$ uniformly w.r.t. $t$

and $\mathcal{L}^{-1}: H^{-\alpha/2} \to H^{\alpha/2}$ continuous + energy identity
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and $L^{-1}: H^{-\alpha/2} \to H^{\alpha/2}$ continuous + energy identity
What about the BC for $\psi$?

**Theorem**

If $\psi \in C^{1,\beta}$, $\beta > 0$, $x_0 \in \partial \Omega$ and

$$\exists n(x_0) = \lim_{\delta \to 0} \delta^{-1-n+\alpha} \iint (x - y)(\varphi_\delta(x) - \varphi_\delta(y))K(x - y)$$

with

$$\varphi_\delta(x) = \left(1 - \delta^{-1}|x - x_0|\right) \chi_{|x-x_0|<\delta}$$

Then $\nabla \psi \cdot n(x_0) = 0$

**Proof:** Local analysis
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Proof: Local analysis
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2. Strain in semiconductors
Main problem

How strain affects electronic properties of semiconductors? How this is reflected in the efficiency of solar cells? Can we tackle the problem from a macroscopic point of view?

- The problem is particularly important for thin films electronics
- We consider crystalline Si for simplicity. More precise models should consider polycrystalline or amorphous Si
Modelling electronic properties

What happens when two differently doped SCs are brought together?

- Charges **diffuse** through the contact
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![Diagram showing charges and electric field](image)
Modelling electronic properties

What happens when two differently doped SCs are brought together?

- Charges diffuse through the contact
- An electric field is built up across the junction and drifts the carriers.

\[ J_n = -q\mu_n n \nabla \psi + qD_n \nabla n \]
\[ J_p = -q\mu_p p \nabla \psi - qD_p \nabla p \]

- \( n \): density of electrons
- \( p \): density of holes
- \( E \): energy of bands
- \( \psi \): electric potential
Strain dependencies

Adding Gauss law and conservation of charges, at equilibrium

\[
\begin{align*}
\epsilon_s \Delta \psi &= q ((n - N_D) - (p - N_A)) \\
0 &= D_n \Delta n - \mu_n \nabla n \cdot \nabla \psi - \mu_n n \Delta \psi + G_n - R_n \\
0 &= D_p \Delta p + \mu_p \nabla p \cdot \nabla \psi + \mu_p p \Delta \psi + G_p - R_p
\end{align*}
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Strain effects

- energy band levels
  \(\rightarrow\) changes in the equilibrium distributions of the charges
- mobilities and diffusivities
  \(\rightarrow\) changes in the conductivity of the material
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- shift in band levels $\rightarrow$ energy gap
- change in shape (multi-valley model + Luttinger Hamiltonian)
Strain dependencies

- shift in band levels $\rightarrow$ energy gap
- change in shape (multi-valley model $+$ Luttinger Hamiltonian)

\[
\begin{align*}
\text{Conduction} & \quad [0, 0, 1] \quad \rightarrow \quad [0, 1, 0] \\
& \quad [1, 0, 0]
\end{align*}
\]

\[
\begin{align*}
\text{Valence} & \quad [0, 0, 1] \quad \rightarrow \quad [0, 1, 0] \\
& \quad [1, 0, 0]
\end{align*}
\]
Strain dependencies

- shift in band levels $\rightarrow$ energy gap
- change in shape (multi-valley model + Luttinger Hamiltonian)
  $\rightarrow$ changes mobilities and effective density of states
The characteristic curve for strained p-n junctions

A p-n junction is the juxtaposition of a n- and a p-doped region. The I-V curve can be obtained by physical arguments or rigorous asymptotic expansions.

- exponential profile in the depletion zone
- injected minority carriers $n^0_p, p^0_n$
- holes and electron currents

$$J \propto \left( n^0_p \sqrt{\frac{D_n}{\tau_n}} + p^0_n \sqrt{\frac{D_p}{\tau_p}} \right) \left( e^{\phi_e/U_T} \right)$$

awaiting for experimental confirmation
Experimental campaign

personal communication, D.Lange LMS–PICM

Experimental setting

n-doped Si

Evidence \(\rightarrow\) Linear(?) behaviour, but combined effect of

- mobility
- change in carrier concentrations
Experimental campaign

personal communication, D. Lange LMS–PICM

Experimental setting

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Energetic formulation and coupling

Bosia, Constantinescu, Jabbour, Triantafyllidis - in preparation

Is a variational formulation of the DD system possible? Nontrivial (the existence proofs require fixed point arguments)

Results

- energetic formulation for DD
- the two transport mechanisms recovered introducing a special internal energy
- coupled model for linear elasticity
- formal and rigourous asymptotic expansions (ongoing work)

Backward coupling can be neglected at first approximation (Maxwell stresses)
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A variational formulation of the DD equations

Internal variables and internal energy

\[ n \quad p \quad \phi \quad \Psi(n, p, \psi) \]

We assume the following dissipation inequality

\[ \frac{d}{dt} \int_{\Omega} \Psi(n, p, \psi) \leq \int_{\Omega} \mathbf{J} \cdot \mathbf{e} - \int_{\partial \Omega} \varphi_n \mathbf{j}_n \cdot \mathbf{n} - \int_{\partial \Omega} \varphi_p \mathbf{j}_p \cdot \mathbf{n} \]

A direct computation gives

\[ \varphi_n = \frac{\partial \psi}{\partial n} \quad \varphi_p = \frac{\partial \psi}{\partial p} \]

\[ -\mathbf{j}_n \cdot (-q \mathbf{e} - \nabla \varphi_n) - \mathbf{j}_p \cdot (q \mathbf{e} - \nabla \varphi_p) \leq 0 \]
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Constitutive equations

Currents

\[ j_n = \frac{\mu_n n}{q} (-q \mathbf{e} - \nabla \varphi_n) \quad j_p = \frac{\mu_p p}{q} (q \mathbf{e} - \nabla \varphi_p) \]

\[ \mu_n \geq 0 \quad \mu_p \geq 0 \]

Internal energy

\[ \Psi = n(\varphi_{n0} - k_B \theta) + k_B \theta n \ln n + p\text{-terms} \]

For the coupled case:

- additional internal variable \( u \)
- \( \mu = \mu(\nabla u) \) and equilibrium equation
Constitutive equations

Currents

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For the coupled case:

- additional internal variable \( u \)
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Towards asymptotics (1D)

Inspired by P. Markowich ’84
- reduced (bulk) equation

\[ 0 = (n - N_D) - (p - N_A) \quad u' = \text{const} \]

- no boundary layer at the (Ohmic) contacts
- computations for the inner layer in progress...
Further developments

Binary fluids
- convergence to stationary states for NSCHO model
- full regularity theory for the nonlocal CH equation
- well-posedness for the nonlocal model $H$ (singular kernel)

Strained electronics
- experimental validation
- asymptotics at the strained p-n junction
- light absorption
- optimisation of strained devices
High cycle fatigue and dynamical systems

Contents

3 High cycle fatigue and dynamical systems
Main problem

We look for a (simple) local rule:

\[ \Phi(\epsilon, \epsilon^p, \sigma, \ldots; \sigma_Y, \ldots) = N_f(x) \quad (or T_f(x)) \]

Reaching the fatigue limit in one point corresponds to crack initiation from that point.

The **time to crack initiation** will be the lowest time to failure of the structure:

\[ N_f = \inf_{x \in \Omega} N_f(x) \]
A macro-meso approach

One active slip system on the most sollicitate grain
Macro- and mesoscopic resolved shear stresses

\[ T = (m \otimes n : \Sigma)m \]
\[ \tau = (m \otimes n : \sigma)m \]
\[ \tau = T - \mu \gamma^p m \]

The active slip system is such that
\[ \tau_{\text{max}} = \max_{n,m} \tau |(m,n)| \]

Dang Van criterion:
Elastic shakedown at both macro- and mesoscales for infinite lifetime

\[ \tau_{\text{max}} + Ap_{\text{max}} \leq B \]
A macro-meso approach

Elastic laws
\[ \sigma = l \varepsilon \quad \Sigma = L E \]
Lin-Taylor scheme
\[ l = L \quad \varepsilon = E \]

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Macro- and mesoscopic resolved shear stresses
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Morel’s model & dynamical systems
Isotropic and kinematic hardening in the inclusion

Von Mises relation:
$$f(\tau, b, \tau_y) = (\tau - b) \cdot (\tau - b) - \tau_y^2$$

Cumulated plastic mesostrain drives hardening
$$\dot{\Gamma} = \sqrt{\dot{\gamma}_p \cdot \dot{\gamma}_p}$$

Constitutive relations

$$\dot{b} = c \dot{\gamma}_p$$
$$\dot{\tau}_y = f(\Gamma) \dot{\Gamma}$$

Diagram:
- $\tau_y$: von Mises stress
- $\tau_{\text{lim}}$: limiting stress
- $\tau_y^{(0)}$: initial yield stress
- $\Gamma$: hardening parameter
- Failure point

Regions I, II, III indicate different stages of material behavior.
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\end{align*} \]
\[ \begin{align*}
\dot{\Gamma} &= \frac{4}{\mu + c + g(\Gamma)} \left( \frac{\Delta T}{2} - G(\Gamma) \right) \\
G(\Gamma) &= \frac{\Delta T_0}{2} - \frac{|\Gamma - \Gamma_0|^\alpha}{\beta} \\
\end{align*} \]
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\[ \dot{y} = y^2 + \epsilon \]

\[ \epsilon > 0 \]

\[ \dot{\gamma}^p = \gamma^p \cdot \dot{\gamma}^p \]

\[ \dot{\gamma} = 4 \frac{\Delta T}{2} - G(\Gamma) \]

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\[ \dot{y} = y^2 + \epsilon \]
\[ \epsilon < 0 \]

\[ \bullet \text{= failure} \]

\[ \tau_y \]
\[ \tau_{\text{lim}} \]
\[ \tau_y^{(0)} \]

I  II  III
Some results

Aluminium 6082 T6


\[ t_{-1} = 92 \text{ MPa} \quad s_{-1} = 132 \text{ MPa} \]

Wohler curve for the data

Observed vs. predicted fatigue endurances