On some multi-phase problems in continuum mechanics

Fluid mixtures—Fatigue—Strained semiconductors

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10th December 2013

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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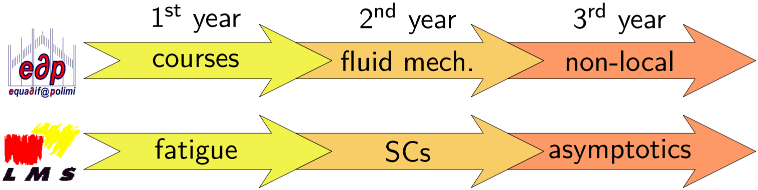


	1st year	2nd year	3rd year
e∂p equa∂if@polimi	courses	fluid mech.	non-local
LMS	fatigue	SCs	asymptotics

Contents

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

Contents

1 Asymptotic behaviour of fluid mixtures

2 Strain in semiconductors

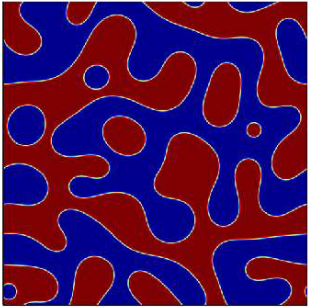
Main problem

Modelling questions:

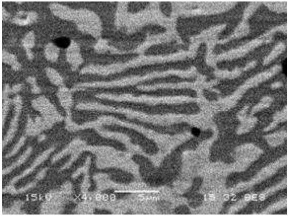
- How can quenching of metals be characterised?
- What can diffuse interface models tell on polymer mixtures?
- How can the insurgent patterns be described?
- Do nonlocal interactions play a significant role?

Mathematical issues:

- Navier-Stokes equations → well-posedness problems in 3D
- physically significant singular potential
- separation property
- regularity theory



Modelling phase separation



Free energy:

$$\Phi = \frac{\epsilon}{2}\int |\nabla\boldsymbol{\psi}|^2 + \frac{1}{\epsilon}\int f(\psi)$$

surface tension double well

A gradient flow approach gives

$$\alpha\partial_t\psi = \Delta(-\epsilon\Delta\psi + \tfrac{1}{\epsilon}f(\psi))$$

α : relaxation parameter

$\sqrt{\epsilon}$: interaction lenght

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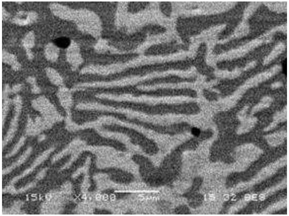

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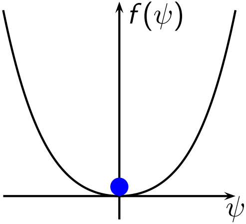
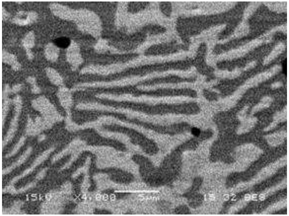


homogeneous phase

Modelling phase separation



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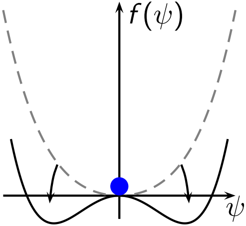

cooling

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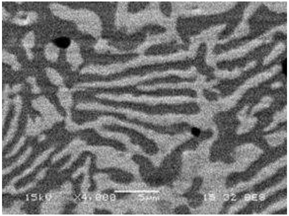

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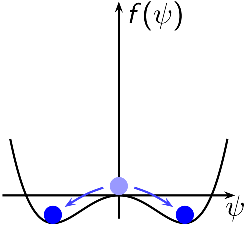

fluctuations → phase separation

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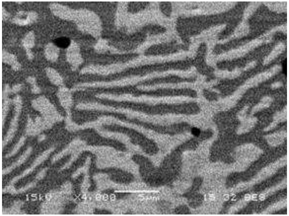

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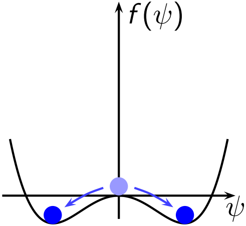
NOT a phase transition!



fluctuations → phase separation

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

$$\int_\Omega \psi(t) = C$$

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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

$$f(\psi) = |\psi|^{2l} - \psi^2$$
$$l \in \mathbb{N}, l \geqslant 2$$

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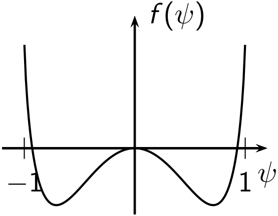

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On nonlocal interactions

Nonlocal interacts between particles of the mixture

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

A hydrodynamic limit leads to the total energy

$$E_P(\psi) \propto \iint_{\Omega\times\Omega} K(|\mathbf{x}-\mathbf{y}|)|\psi(\mathbf{x})-\psi(\mathbf{y})|^2 + \mathrm{O.T.}$$

Regular kernel $K \in W^{1,1}$

- second-order integro-differential equation
- studied by Frigeri, Grasselli et al.

Singular kernel $K(\mathbf{y}) \propto |\mathbf{y}|^{-n-\alpha}$

- formal structure of CH equation preserved
- incomplete regularity theory

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The Cahn-Hilliard-Navier-Stokes system

$\Omega \in \mathbb{R}^n,\ n = 2, 3$

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

Main assumptions

- stress-deformation rate relation
- chemical potential

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

- diffusion operator

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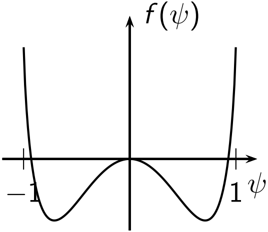

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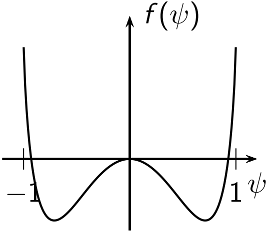

- diffusion operator

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 $\{S(t)\}_{t \geqslant 0}$, $S(t) \colon X \to X$ is a semigroup on X if

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

Definition

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

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Theorem

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

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

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If $\{S(t)\}_{t \geqslant 0}$ 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
  → existence, trajectory attractor
- chemically reacting fluids, 2D regular potential
  → well-posedness, robust family of exponential attractors
- original system, potential with arbitrary polynomial growth
  → pullback exponential attractor
- nonlocal diffusion
  → existence, regularity

Non-newtonian fluids

Bosia - J. Math. Anal. Appl. **397**, 307–321 (2012)

Shear-thickening fluid

$$\boldsymbol{\tau}(\nabla \mathbf{u}) : \nabla \mathbf{u} \geqslant C_N \left|\nabla \mathbf{u}\right|^2 + C_L \left|\nabla \mathbf{u}\right|^p$$

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

Bosia, Grasselli, Miranville - Math. Methods Appl. Sci. (2013)

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

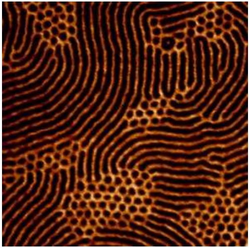
$$\partial_t \psi + (\mathbf{u} \cdot \nabla)\psi + \delta(\psi - c_0) = \Delta\mu$$

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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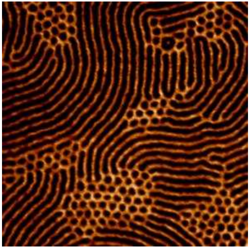

Exponential pullback attractors

Bosia, Gatti - submitted

The pullback attracting property can be written as

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

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)
- non-autonomous forcing term

Results

- existence
- regularity estimates depending on the growth of the potential only through constants
- existence of an exponential pullback attractor

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Nonlocal interactions

Abels, Bosia, Grasselli - submitted

The chemical potential is given by

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

$\mathcal{E}$ is the "regional fractional laplacian"

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

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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Nonlocal interactions II

Existence and uniqueness

Theorem

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

$$\psi \in \mathbf{C}(H^{\alpha/2}_{(0)}) \qquad \partial_t \psi \in L^2(H_0^{-1}) \qquad \mu \in L^2(H^1)$$

Moreover there hold

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

$$\text{if } n \leqslant 3 \quad \psi \in L^\infty(\mathbf{C}^\beta) \quad \text{for some } \beta > 0$$

and the associated semigroup has a (connected) global attractor

WARNING! The expected $L^2(H^\alpha)$ regularity is unknown

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Moreover there hold

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

$$\textit{if } n \leqslant 3 \quad \psi \in L^\infty(\mathbf{C}^\beta) \quad \textit{for some } \beta > 0$$

and the associated semigroup has a (connected) global attractor

WARNING! The expected $L^2(H^\alpha)$ regularity is unknown

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

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

and $\mathcal{L}^{-1}: H^{-\alpha/2} \to H^{\alpha/2}$ continuous + energy identity

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Nonlocal interactions III

On the boundary conditions

What about the BC for ψ?

Theorem

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

$$\exists \mathbf{n}(\mathbf{x}_0) = \lim_{\delta \to 0} \delta^{-1-n+\alpha} \iint (\mathbf{x}-\mathbf{y})(\varphi_\delta(\mathbf{x}) - \varphi_\delta(\mathbf{y}))K(\mathbf{x}-\mathbf{y})$$

with

$$\varphi_\delta(\mathbf{x}) = \left(1 - \delta^{-1}|\mathbf{x}-\mathbf{x}_0|\right) \chi_{|\mathbf{x}-\mathbf{x}_0|<\delta}$$

Then $\nabla\psi \cdot \mathbf{n}(\mathbf{x}_0) = 0$

Proof: Local analysis

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Proof: Local analysis

Contents

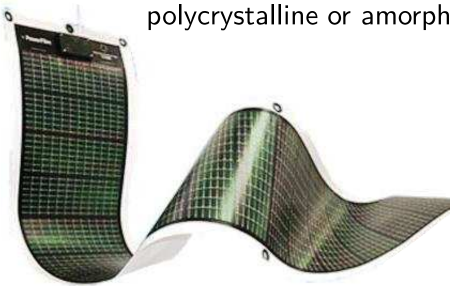
1 Asymptotic behaviour of fluid mixtures

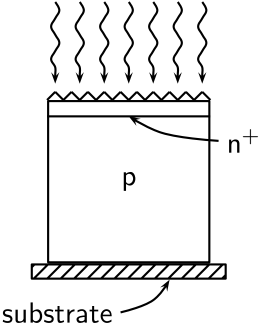
2 Strain in semiconductors

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

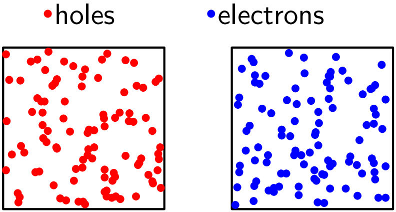




Modelling electronic properties

What happens when two differently doped SCs are brought together?

- Charges diffuse through the contact
- An electric field is build up across the junction



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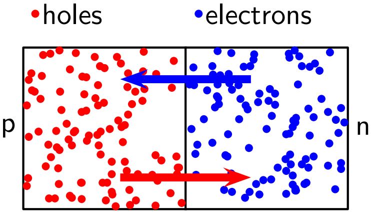

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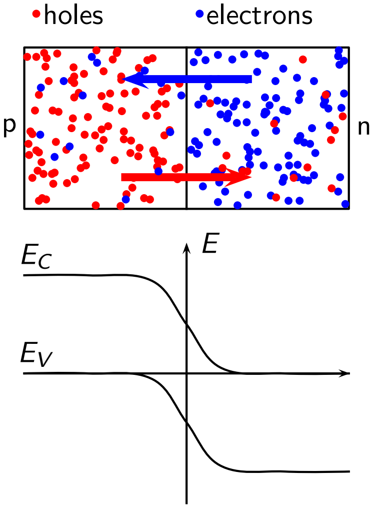


Modelling electronic properties

What happens when two differently doped SCs are brought together?

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

$$\mathbf{J}_n = -q\mu_n \, n \nabla\psi + qD_n \nabla n$$

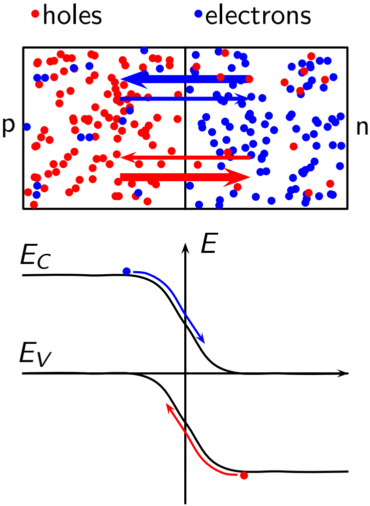
$$\mathbf{J}_p = -q\mu_p \, p \nabla\psi - qD_p \nabla p$$

n: density of electrons

p: density of holes

E: energy of bands

ψ: electric potential



Strain dependencies

Adding Gauss law and conservation of charges, at equilibrium

$$\begin{cases} \epsilon_s \Delta\psi = q\left((n - N_D) - (p - N_A)\right) \\ 0 = D_n \Delta n - \mu_n \nabla n \cdot \nabla\psi - \mu_n n \Delta\psi + G_n - R_n \\ 0 = D_p \Delta p + \mu_p \nabla p \cdot \nabla\psi + \mu_p p \Delta\psi + G_p - R_p \end{cases}$$

Strain effects

- energy band levels
  → changes in the equilibrium distributions of the charges
- mobilities and diffusivities
  → changes in the conductivity of the material

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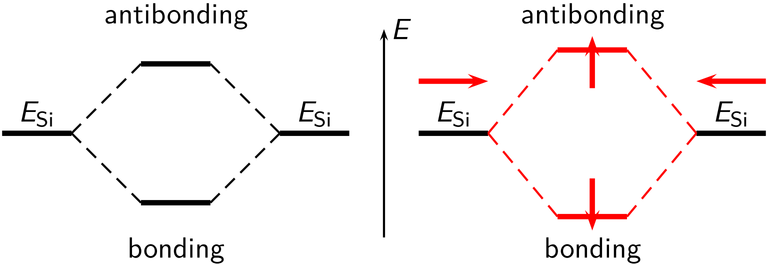
- shift in band levels → energy gap
- change in shape (multi-valley model + Luttinger Hamiltonian)



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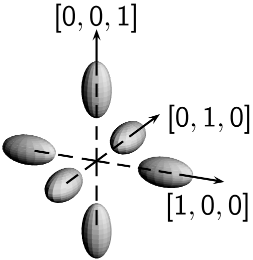
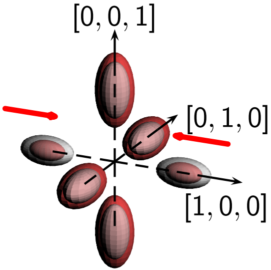
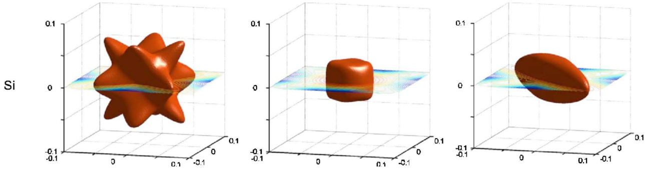
Conduction band





Valence band



unstressed

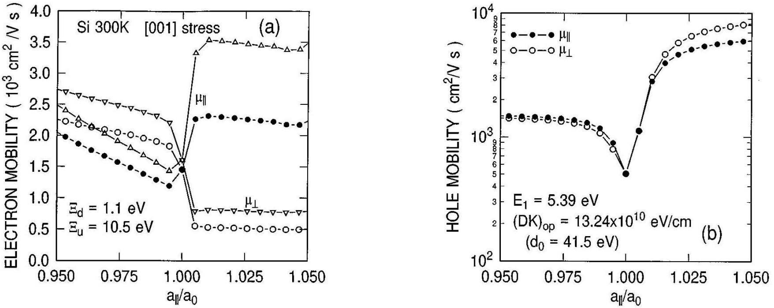
1GPa biaxial tensile

1GPa uniaxial compressive

Strain dependencies

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

→ changes mobilities and effective density of states

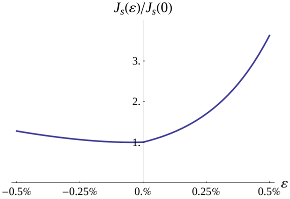


The characteristic curve for strained p-n junctions

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 rigourous asymptotic expansions

- exponential profile in the depletion zone
- injected minority carriers n_p^0, p_n^0
- holes and electron currents

$$J \propto \left(n_p^0 \sqrt{\frac{D_n}{\tau_n}} + p_n^0 \sqrt{\frac{D_p}{\tau_p}} \right) \left(e^{\phi_e / U_T} \right)$$



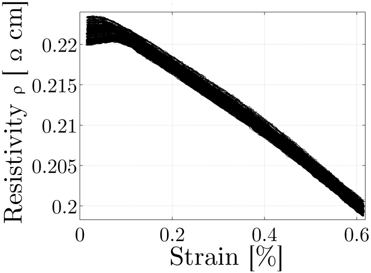
awaiting for experimental confirmation

Experimental campaign

personal communication, D.Lange LMS–PICM

Experimental setting

n-doped Si



Evidence → Linear(?) behaviour, but combined effect of

- mobility
- change in carrier concentrations

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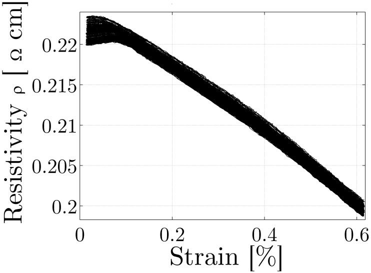

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Energetic formulation and coupling

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

$$n \quad p \quad \phi \qquad \Psi(n, p, \psi)$$

We assume the following dissipation inequality

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_\Omega \Psi(n, p, \psi) \leqslant \int_\Omega \mathbf{J} \cdot \mathbf{e} - \int_{\partial\Omega} \varphi_n \mathbf{j}_n \cdot \nu - \int_{\partial\Omega} \varphi_p \mathbf{j}_p \cdot \nu$$

A direct computation gives

$$\varphi_n = \frac{\partial \Psi}{\partial n} \qquad \varphi_p = \frac{\partial \Psi}{\partial p}$$

$$-\mathbf{j}_n \cdot (-q\mathbf{e} - \nabla \varphi_n) - \mathbf{j}_p \cdot (q\mathbf{e} - \nabla \varphi_p) \leqslant 0$$

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Constitutive equations

Currents

$$\mathbf{j}_n = \frac{\mu_n n}{q}\left(-q\mathbf{e} - \nabla\varphi_n\right) \qquad \mathbf{j}_p = \frac{\mu_p p}{q}\left(q\mathbf{e} - \nabla\varphi_p\right)$$

$$\mu_n \geqslant 0 \qquad \mu_p \geqslant 0$$

Internal energy

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

For the coupled case:

- additional internal variable $\mathbf{u}$
- $\mu = \mu(\nabla\mathbf{u})$ and equilibrium equation

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Towards asymptotics (1D)

Inspired by P.Markowich '84

- reduced (bulk) equation

$$0 = (n - N_D) - (p - N_A) \qquad u' = const$$

- 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

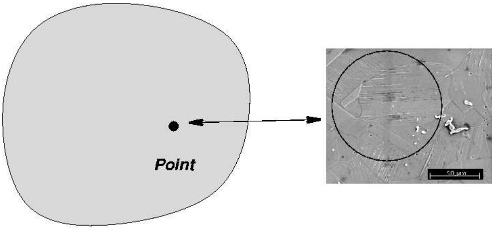
Contents

3 High cycle fatigue and dynamical systems

Main problem

We look for a (simple) local rule:

$$\Phi(\epsilon, \epsilon^{p}, \boldsymbol{\sigma}, \ldots; \boldsymbol{\sigma}_{Y}, \ldots) = N_f(\mathbf{x}) \quad (or T_f(\mathbf{x}))$$



Mathematical point

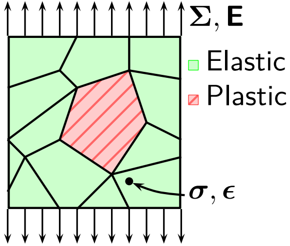
Physical microstructure

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

$$N_f = \inf_{\mathbf{x} \in \Omega} N_f(\mathbf{x})$$

A macro-meso approach



Elastic laws

$$\boldsymbol{\sigma} = \mathbf{l}\boldsymbol{\epsilon} \quad \boldsymbol{\Sigma} = \mathbf{L}\mathbf{E}$$

Lin-Taylor scheme

$$\mathbf{l} = \mathbf{L} \qquad \boldsymbol{\epsilon} = \mathbf{E}$$

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

$$\tau_{\mathrm{max}} + Ap_{\mathrm{max}} \leqslant B$$

One active slip system on the most sollicitate grain

Macro- and mesoscopic resolved shear stresses

$$\mathbf{T} = (\mathbf{m} \otimes \mathbf{n} : \boldsymbol{\Sigma})\mathbf{m}$$

$$\boldsymbol{\tau} = (\mathbf{m} \otimes \mathbf{n} : \boldsymbol{\sigma})\mathbf{m}$$

$$\boldsymbol{\tau} = \mathbf{T} - \mu\gamma^p\mathbf{m}$$

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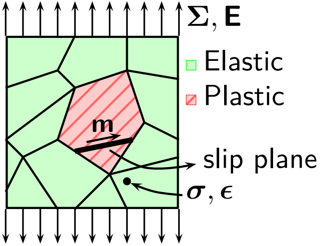

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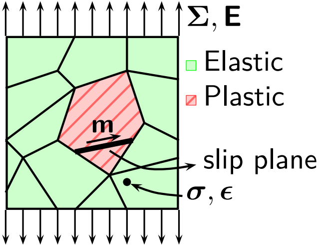

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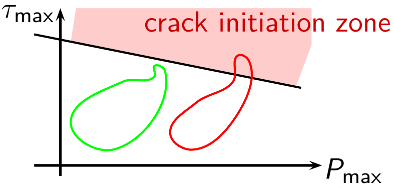

Morel's model & dynamical systems

Isotropic and kinematic hardening in the inclusion

Morel - Fat. & Fract. of Eng. Mat. & Struct. **21**, 241–256 (1998)

Von Mises relation:

$$f(\boldsymbol{\tau}, \mathbf{b}, \tau_y) = (\boldsymbol{\tau} - \mathbf{b}) \cdot (\boldsymbol{\tau} - \mathbf{b}) - \tau_y^2$$

Cumulated plastic mesostrain drives hardening

$$\dot{\Gamma} \doteq \sqrt{\dot{\gamma}^p \cdot \dot{\gamma}^p}$$

Constitutive relations

$$\dot{\mathbf{b}} = c\dot{\gamma}^p$$
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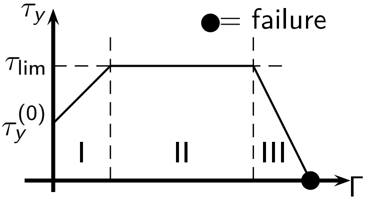

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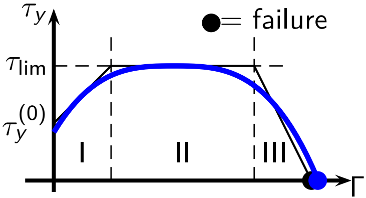

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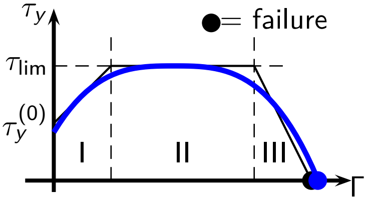
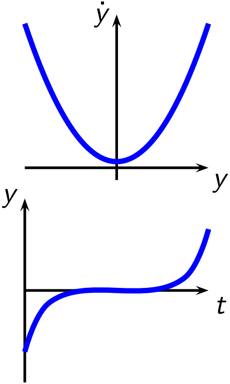


$$\dot{y} = y^2 + \epsilon$$

$$\epsilon > 0$$



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Von Mises relation:

$$f(\boldsymbol{\tau}, \mathbf{b}, \tau_y) = (\boldsymbol{\tau} - \mathbf{b}) \cdot (\boldsymbol{\tau} - \mathbf{b}) - \tau_y^2$$

Cumulated plastic mesostrain drives hardening

$$\dot{\Gamma} \doteq \sqrt{\dot{\gamma}^p \cdot \dot{\gamma}^p}$$

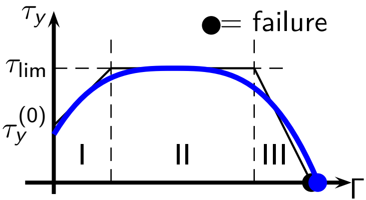
Constitutive relations

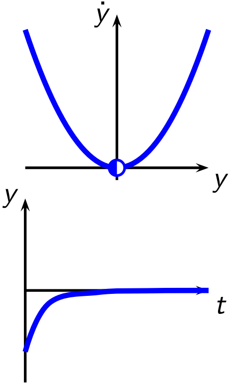
$$\dot{\mathbf{b}} = c\dot{\gamma}^p \qquad \dot{\Gamma} = \frac{4}{\mu+c+g(\Gamma)}\left(\frac{\Delta T}{2} - G(\Gamma)\right)$$

$$\dot{\tau_y} = f(\Gamma)\dot{\Gamma} \qquad G(\Gamma) = \frac{\Delta T_0}{2} - \frac{|\Gamma-\Gamma_0|^\alpha}{\beta}$$

$$\dot{y} = y^2 + \epsilon$$

$$\epsilon = 0$$





Morel's model & dynamical systems

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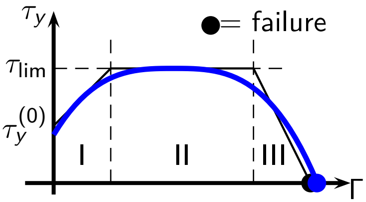
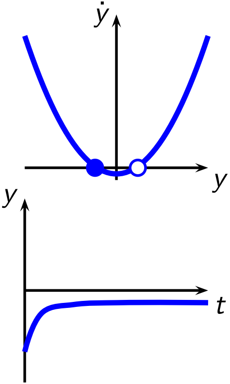


$$\dot{y} = y^2 + \epsilon$$

$$\epsilon < 0$$



Some results

Aluminium 6082 T6

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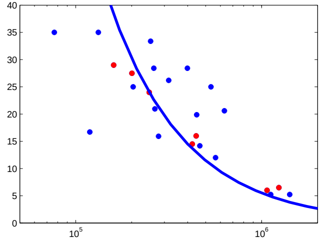
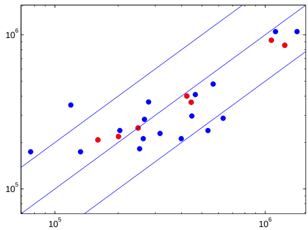
$$t_{-1} = 92\,\mathrm{MPa} \qquad s_{-1} = 132\,\mathrm{MPa}$$



Wohler curve for the data



Observed vs. predicted fatigue endurances