A two scale model for liquid phase epitaxy with elasticity

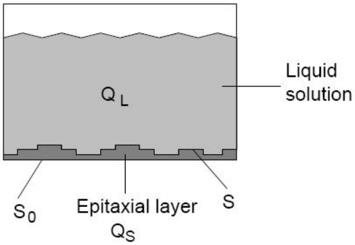
Ch. Eck, M. Kutter, Ch. Rohde, A.-M. Sändig

Institute of Applied Analysis and Numerical Simulation
University of Stuttgart

12. International Conference on
Free Boundary Problems
Theory and Applications

Chiemsee, June 11-15, 2012

Liquid phase epitaxy



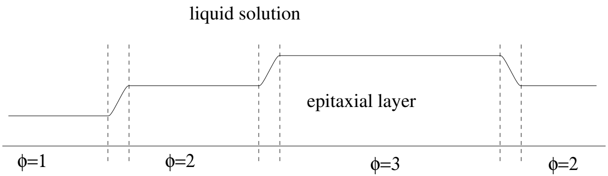
- Molecules are solved in the liquid solution
- Epitaxial layer grows on a substrate
- Elastic deformations in the layer

Two scale model [Eck/Emmerich]:

In the liquid	On the surface	In the layer
convection diffusion	adsorption/desorption surface diffusion incorporation of moleculs	elastic effects

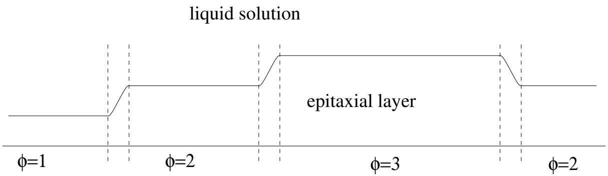
Phase field approximation

The phase field ϕ represents the number of monomolecular layers over a point on S_0.

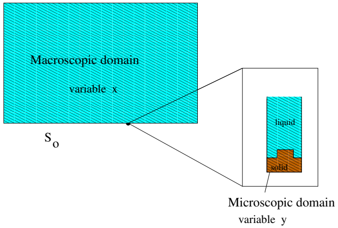


Phase field approximation

The phase field ϕ represents the number of monomolecular layers over a point on S_0.



Two scale formulation



Macro:

- Transport in the liquid

Micro:

- Transport in the liquid
- Evolution of the interface
- Elastic effects

Microscopic Equations I

For the phase field ϕ and the surface concentration c^S:

$$\left.\begin{aligned} \alpha\xi^2\partial_t\phi - \xi^2\Delta_y\phi + f'(\phi) + q(c^S, u, \phi) = 0, \\ \partial_t c^S + \varrho_S h_A \partial_t\phi - D_S\Delta_y c^S = \frac{C^V}{\tau_V} - \frac{c^S}{\tau_S}, \end{aligned}\right\} \quad \text{in } Y,$$

where

- Y: 2D-periodicity cell,
- f: multi-well potential with minima at integer values,
- C^V: volume concentration of molecules in the liquid,
- u: mechanical displacement field in the layer,
- q: surface energy density on the interface.

$+$ periodic boundary conditions,

$+$ initial conditions.

Microscopic Equations II

For the fluid velocity v and pressure p:

$$\begin{aligned} \operatorname{div}_y v &= 0, \quad \text{in } Q_l, \\ -\eta\Delta_y v + \nabla_y p &= 0, \quad \text{in } Q_l, \\ v &= -J_S^{-1}\left(\tfrac{1}{\varrho_V}-\tfrac{1}{\varrho_E}\right)\left(\tfrac{c^V}{\tau_V}-\tfrac{c^S}{\tau_S}\right)e_3 \quad \text{on } \Gamma, \end{aligned}$$

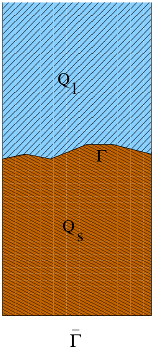
matching condition for $y_3 \to \infty$.

For the displacement field u:

$$\begin{aligned} -\operatorname{div}_y \sigma_y(u) &= 0, \quad \text{in } Q_s. \\ u &= b, \quad \text{on } \bar{\Gamma}, \\ \left(\sigma_y(u)+\eta(\nabla_y v+(\nabla_y v)^\top)-p\mathbf{I}\right)\vec{n} &= 0, \quad \text{on } \Gamma, \end{aligned}$$

where $\sigma_y(u)=\mathbf{c}e_y(u)$, $e_y(u)=\frac{1}{2}(\nabla u+(\nabla u)^\top)$.

$+$ periodic boundary conditions for y_1, y_2.



Macroscopic Equations

For the fluid velocity V, pressure P and the volume concentration C^V:

$$\begin{aligned} \operatorname{div}_x V &= 0, \\ \partial_t V + (V \cdot \nabla_x) V - \eta \Delta_x V + \nabla_x P &= 0, \\ \partial_t C^V + V \cdot \nabla_x C^V - D_V \Delta_x C^V &= 0. \end{aligned}$$

Coupling conditions to the microscopic problems:

$$\left. \begin{aligned} D_V \partial_{x_3} C^V|_{x_3=0} &= \left(\frac{C^V}{\tau_V} - \frac{\bar{c}^S}{\tau_S} \right), \\ V &= 0, \end{aligned} \right. \qquad \text{on } S_0.$$

(+ initial conditions and boundary conditions on the rest of the boundary.)

Here, $\bar{c}^S(t,x) = \int_Y c^S(t,x,y)\,\mathrm{d}y$.

The Navier-Stokes equations decouple from the other equations.

Solvability of the single models

Consider the coupling data as given. Then each single problem has a unique solution:

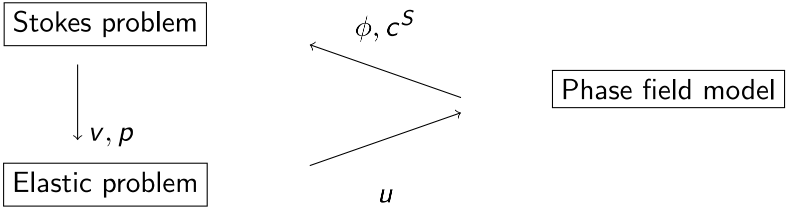
Problem	Coupling data	Unknowns
Stokes	$\phi \in C^2(\bar{Y})$ $c^S \in W^{2-1/r,r}(Y)$	$v \in W^{2,r}_{\mathrm{loc}}(Q_l)$ $p \in W^{1,r}_{\mathrm{loc}}(Q_l)$
Elasticity	$v \in W^{2,r}_{\mathrm{loc}}(Q_l)$ $p \in W^{1,r}_{\mathrm{loc}}(Q_l)$ $\phi \in C^2(\bar{Y})$	$u \in W^{2,r}(Q_s)$
Phase field	$u \in W^{2,r}(Y)$ $C^V \in L^2(I)$	$\phi \in L^2(I, W^{3-1/r,r/2}(Y))$ $c^S \in L^2(I, W^{3-1/r,r/2}(Y))$
Convection-diffusion	$\bar{c}^S \in L^2(I \times S_0)$	$C^V \in L^2(I, H^1(Q))$

with $r > 5$.

Future work

Fixed point approach

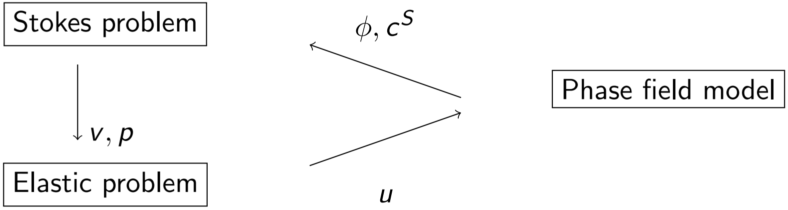
Microscopic coupling:



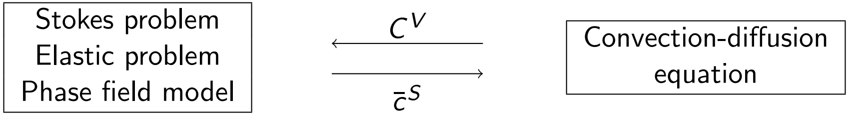
Future work

Fixed point approach

Microscopic coupling:



Micro-macro coupling:



Conclusion and Outlook

Conclusion:

- Two scale model for liquid phase epitaxy with elasticity,
- Analytical results.

Outlook:

- Solvability of the fully coupled problem,
- Justification of the two scale approach.

Thank you for your attention.

DFG Support of the German Research Foundation is gratefully acknowledged.