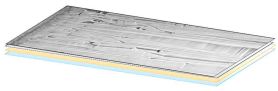
Freie Universität Berlin
www.fu-berlin.de

NONSMOOTH SCHUR NEWTON METHOD FOR A MULTIPHASE FIELD MODEL OF THE LIQUID PHASE CRYSTALLIZATION PROCESS

Max Kahnt, Ralf Kornhuber

HELMHOLTZ GEMEINSCHAFT
HVI *Microstructure control for thin film solar cells*

LPC process



Device layers

Nano-crystalline silicon is evaporated onto base layers and sealed with capping layers. Each layer has to provide good efficiency and producibility properties. The device is then swept over by a line shaped heat source (e.g. laser) to create a coarser, more favorable silicon absorption layer after re-crystallization. It exhibits larger grains that are mostly columnar in the thin film direction.

In our simulation we consider the melting and recrystallization process of the silicon layer.

Grains after sweeping from left

Multiphase model

$$S(e,\phi) = \int s - \epsilon\gamma^2 - \tfrac{1}{\epsilon}\Psi \,\mathrm{d}x \qquad \text{entropy functional}$$

Thermodynamical assumptions:

$$\mathrm{d}f = -s\,\mathrm{d}T + \sum \frac{\partial f}{\partial \phi_\alpha}\,\mathrm{d}\phi_\alpha \qquad \text{Gibbs relation}$$

$$e = f + sT \qquad \text{energy contributions}$$

Evolution principles:

$$\epsilon\partial_t\phi_\alpha = \frac{\delta S}{\delta\phi_\alpha} - \lambda \qquad \text{scaled gradient flow}$$

$$\partial_t e = -\nabla\cdot\beta(T,\phi)\nabla\frac{\delta S}{\delta e} \qquad \text{energy conservation}$$

internal energy density e, internal entropy density s, free energy density f, temperature T, phases ϕ_α, diffuse interface' thickness ϵ, phase anisotropy γ, phase separation Ψ, Lagrange multiplier λ, flow coeff. β

Coupled phase-temperature problem with constraints

We choose $f = \sum L_\alpha \frac{T-T_\alpha}{T_\alpha}\phi_\alpha - c_v T(\log T - 1)$, isotropic phase gradients and a double-well potential to drive the phase separation. Natural boundary conditions for the phases are employed and the heating effect of the laser as well as the steady environmental cooling is modeled by convection. The observation of columnar growth in the thin film LPC process motivates further assumptions that allow the reduction to 2D. We formulate the problem in inverse temperature $\theta = \frac{1}{T}$ and end up with the coupled nonlinear variational inequality

$$\epsilon(\partial_t\phi, v-\phi) + \epsilon(\nabla\phi,\nabla(v-\phi)) - \tfrac{1}{\epsilon}\chi(v) + \tfrac{1}{\epsilon}\chi(\phi) \le (\tfrac{1}{\epsilon}K\phi - L\theta + La + \mathbb{1}\lambda, v-\phi)$$
$$(\partial_t(c_v\tfrac{1}{\theta} - L^T\phi), v) - (\beta\nabla\theta,\nabla v) + (Q\tfrac{1}{\theta}, v) = (QT_B, v)$$
$$(\mathbb{1}^T\phi, v) = (1, v)$$

The first inequality governs the phase evolution constrained to non-negative values. The second equation describes the temperature coupled to the change in phases and heating resp. cooling from the exterior. The third equation enforces the sum-constraint.

Discretization:

- Linearly semi-implicit Euler
- Linear finite elements

latent heats L and inverse melting temperatures a, indicator function χ, double-well potential derivative $K\phi$, ambient temperature T_B with convection coefficient Q

Nonsmooth Schur Newton method and TNNMG

Nonlinear saddle point	Find root	Minimization
$\begin{pmatrix} F & B^T \\ B & -C \end{pmatrix}\begin{pmatrix}\phi \\ w\end{pmatrix} \ni \begin{pmatrix} f \\ g\end{pmatrix}$	$H(w) = 0$	$w = \arg\min_v h(v)$

All three problems are equivalent for $w = \binom{\theta}{\lambda}$ and $\phi = F^{-1}(f - B^T w)$.

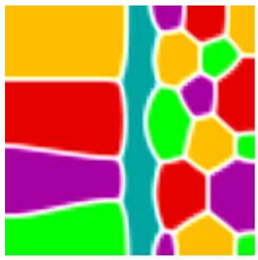
A descent method for the unconstrained minimization problem is applied. The descent directions are chosen in analogy to Newton's method albeit using a generalized second derivative to handle the non-smoothness.

In each step, ϕ has to be determined by inverting F which can be done efficiently using truncated nonsmooth Newton multigrid (TNNMG). Descent directions are computed by solving a linear saddle point problem. Convergence towards the solution is achieved by choosing efficient step sizes.

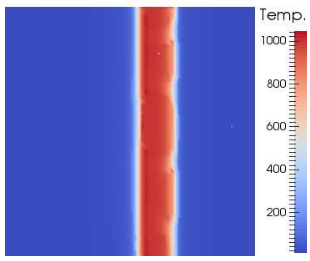
$H(w) = -B\phi + Cw + g$ and $h = -\mathcal{L}(F^{-1}(f - B^T w), w)$ with $\nabla h = H$.

Numerical simulation

A snapshot of the phase evolution is shown. Each color represents a distinct grain where ■ is liquid; ■, ■, ■ and ■ crystals.



A temperature of 1000K is induced by the laser sweeping over the domain from left to right.



Small grains on the right side vanish when being passed by the laser. Recrystallized grains evolve from the left.

References

Pictures for LPC process kindly provided by Dr.-Ing. Daniel Amkreutz

Stinner, Nestler, and Garcke. *A diffuse interface model for alloys with multiple components and phases.* SIAM Journal o. Appl. Math. 64.3 (2004): 775-799.

Gräser, and Kornhuber. *Nonsmooth Newton methods for set-valued saddle point problems.* SIAM Journal on Numer. Anal. 47.2 (2009): 1251-1273.

Gräser, Sack, and Sander. *Truncated nonsmooth Newton multigrid methods for convex minimization problems.* DDM. in SaE. XVIII., 2009. 129-136.

Implementation in DUNE (`dune-project.org`); Visualization with Paraview (`paraview.org`)