EVOLUTION OF ELASTIC THIN FILMS WITH CURVATURE REGULARIZATION VIA MINIMIZING MOVEMENTS

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Abstract : the evolution equation with curvature regularization that models the motion of a two-dimensional thin film by evaporation-condensation on a rigid substrate is considered. The film is strained due to a mismatch between the crystalline lattices of the two materials. Short time existence, regularity, and uniqueness of the solution are established using De Giorgi's minimizing movements to exploit the L^2-gradient flow structure of the equation. This seems to be the first analytical result for the evaporation-condensation case in the presence of elasticity.

Epitaxy

Consider the deposition of film atoms

- on a rigid substrate,
- in the presence of a mismatch between the crystalline lattices,
- with the profile modeled as a grain-vapor anisotropic interface,
- in the evaporation-condensation process.

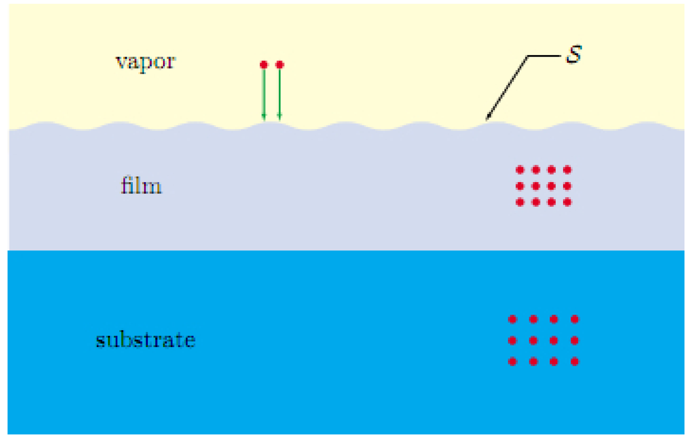


FIGURE: Epitaxy, courtesy of Fried and Gurtin (2004).

Two mechanisms determine the profile of the film :

- lattice mismatch ⇒ elastic energy
  ⇒ migration of film atoms
  ⇒ undulations, isolated islands, ...
- non-flat profiles are less convenient with respect to surface energy.

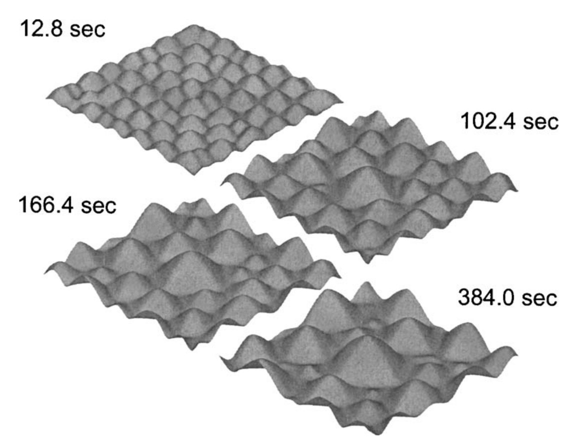
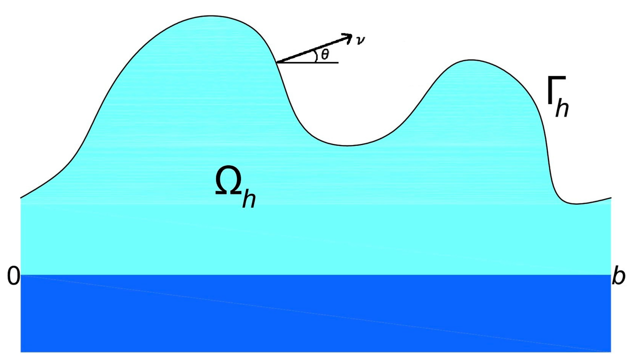


FIGURE: ATG instability. Simulation by Wise *et al.* (2005).

Variational Formulation : Configurations and Total Energy

$h:\mathbb{R}\to[0,\infty)$ profile function
$\Gamma_h:=\{(x,h(x)):0<x<b\}$
$u:\Omega_h\to\mathbb{R}^2$ planar displacement
$\Omega_h:=\{(x,y):0<x<b,0<y<h(x)\}$



Admissible configurations (h,u) are :

- b-periodic, i. e., h is b-periodic and u satisfies $u(x+b,y)=u(x,y)+(e_0 b,0)$ for $(x,y)\in\Omega_h^{\#}$,
- $e_0>0$ represents the lattice mismatch,
- $h\in H^2(0,b)$, $u\in H^1(\Omega_h;\mathbb{R}^2)$, and $u(\cdot,0)=(e_0\cdot,0)$.

The total energy of an admissible configuration (h,u) is

$$\mathscr{F}(h,u):=\underbrace{\int_{\Omega_h}W(\boldsymbol{E}(u))\,\mathrm{d}z}_{\text{elastic bulk energy}}+\underbrace{\int_{\Gamma_h}\psi(\nu)\,\mathrm{d}\mathscr{H}^1}_{\text{surface energy}}+\underbrace{\frac{\lambda}{2}\int_{\Gamma_h}k^2\,\mathrm{d}\mathscr{H}^1}_{\text{perturbation}},$$

where

- $\boldsymbol{E}(u):=\frac{1}{2}(\nabla u+(\nabla u)^T)$ represents the strain,
- $W(\boldsymbol{A}):=\frac{1}{2}\mathbb{C}(\boldsymbol{A}):\boldsymbol{A}$ where $\mathbb{C}$ is a positive definite 4^{th}-order tensor,
- $\nu:=$ outer normal vector of Ω_h, $k:=$ curvature of Γ_h, $\lambda>0$,
- the anisotropic surface energy density $\psi:\mathbb{R}^2\to[0,\infty)$ is a positively 1-homogeneous function of class C^2 away from the origin.

Evaporation-Condensation Evolution Equation

$$V=(g_{\theta\theta}+g)k-W(\boldsymbol{E}(u))-\lambda\left(k_{\sigma\sigma}+\tfrac{1}{2}k^3\right)=\text{first variation of }\mathscr{F},$$

where $V=\frac{h_t}{\sqrt{1+h_x^2}}$ is the normal velocity, $g(\theta):=\psi(\cos\theta,\sin\theta)$, and $W(\boldsymbol{E}(u))$ denotes the trace of $W(\boldsymbol{E}(u(\cdot)))$ on $\Gamma_{h(\cdot)}$.

References : Herring (1951) ; Mullins (1956, 1957), Gurtin (1988) ; Gurtin, Struthers (1988) ; Angenent, Gurtin (1989) ; Di Carlo, Gurtin, Podio-Guidugli (1992) ; Gurtin, Soner, Souganidis (1995) ; ...

Previous Results :

- numerical simulations : Rätz, Ribalta, Voigt (2006) ; Burger, Haußer, Stöcker, Voigt (2007) ; Burger, Stöcker, Voigt (2008).
- analytical results concerning L^2-gradient flows (without elasticity) : Bellettini, Mantegazza, Novaga (2007).
- analytical results for the surface diffusion case without evaporation-condensation : Fonseca, Fusco, Leoni, Morini (2012) ; Dal Maso, Fonseca, Fusco, Leoni (2012).

No analytical result for the evaporation-condensation case

Existence (P., *Calc. Var. PDEs*, in press)

There exists $T_0>0$ such that for each $T<T_0$ the Cauchy problem (CP) *admits a solution (h,u) with profile satisfying*
$h\in L^2(0,T;H^4_{\mathrm{loc}}(\mathbb{R}))\cap L^\infty(0,T;H^2_{\mathrm{loc}}(\mathbb{R}))\cap H^1(0,T;L^2_{\mathrm{loc}}(\mathbb{R}))$.

Regularity (P., *Calc. Var. PDEs*, in press)

Let (h,u) be the solution of (CP) *in $[0,T]$ given by the Existence Theorem for $T<T_0$. Then, the profile h satisfies :*

(i) $h\in C^{0,\beta}([0,T];C^{1,\alpha}([0,b]))$ *for every* $\alpha\in\left(0,\frac{1}{2}\right)$ *and* $\beta\in\left(0,\frac{1-2\alpha}{8}\right)$,

(ii) $h\in L^{\frac{12}{5}}(0,T;C^{2,1}([0,b]))\cap L^{\frac{24}{5}}(0,T;C^{1,1}([0,b]))$,

(iii) $\|h_x\|_{L^\infty(0,T;L^\infty(0,b))}\le\|h_0'\|_\infty+\sqrt{\|h_0'\|^2_\infty+1}$.

Uniqueness (P., *Calc. Var. PDEs*, in press)

If (h_1,u_1) and (h_2,u_2) are two solutions of (CP) *in $[0,T]$ with*
$h_1,h_2\in L^2(0,T;H^4_{\mathrm{loc}}(0,b))\cap L^\infty(0,T;H^2_{\mathrm{loc}}(0,b))\cap H^1(0,T;L^2_{\mathrm{loc}}(0,b))$,
then they coincide.

Cauchy Problem

Let $T>0$ and $h_0\in H^2_{\mathrm{loc}}(\mathbb{R};(0,\infty))$ be a b-periodic initial profile.

$$\begin{cases}\frac{h_t}{\sqrt{1+h_x^2}}=(g_{\theta\theta}+g)k-W(\boldsymbol{E}(u))-\lambda\left(k_{\sigma\sigma}+\frac{1}{2}k^3\right)\text{ on }\mathbb{R}\times(0,T)\\ \operatorname{div}\mathbb{C}\boldsymbol{E}(u)=0\text{ in }\Omega_h\\ \mathbb{C}\boldsymbol{E}(u)[\nu]=0\text{ on }\Gamma_h\text{ and }u(x,0,t)=(e_0x,0)\\ (h,u)\text{ is a }b\text{-periodic configuration in }\Omega_h\\ h(\cdot,0)=h_0\end{cases}\qquad\text{(CP)}$$

References : Fried, Gurtin (2004) ; Li, Lowengrub, Rätz,Voigt (2009).

Goals : existence, regularity, uniqueness of solutions of (CP)

Gradient Flow Structure

The evolution equation is the gradient flow of the reduced energy $\mathscr{E}$ with respect to a suitable L^2-metric, i.e.,

$$h_t=-\nabla_{L^2}\mathscr{E}(h),$$

where $\mathscr{E}(h):=\mathscr{F}(h,u_h)$ and u_h is the elastic equilibrium w.r.t. h.

Reference : Cahn, Taylor (1994) in the case without elasticity.

➡ De Giorgi's minimizing movement method

Incremental Minimum Problem

Let (h_0,u_0) be an initial configuration. For $r>\|h_0'\|_\infty$, $T>0$, $N\in\mathbb{N}$, $i=1,\dots,N$, define inductively $(h^r_{i,N},u^r_{i,N})$ as the solution of

$$\min_{\substack{(h,u)\text{ adm.}\\ \text{s.t. }\|h'\|_\infty\le r}}\left\{\mathscr{F}(h,u)+\frac{1}{2\tau_N}\int_{\Gamma_{h^r_{i-1,N}}}\left(\frac{h-h^r_{i-1,N}}{J^r_{i-1,N}}\right)^2\mathrm{d}\mathscr{H}^1\right\}$$

where $\tau_N:=T/N$ and $J^r_{i-1,N}:=\sqrt{1+((h^r_{i-1,N})')^2}$.

There exist r_0 and T_0 s. t. the approximate solutions $h^{r_0}_N$ defined by $h^{r_0}_N(\cdot,t):=h^{r_0}_{i-1,N}+\frac{1}{\tau_N}(t-(i-1)\tau_N)(h^{r_0}_{i,N}-h^{r_0}_{i-1,N})$ for $t\in[(i-1)\tau_N,i\tau_N]$ satisfy $\|(h^{r_0}_N)'\|_\infty<r_0$ and converge to the solution h in $[0,T_0]$.

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