Summary. Epitaxy is a process in which a crystalline over-layer (often referred as "epitaxial film" due to its very low thickness compared to the substrate) is deposited on a crystalline substrate, and the film locks into one or more crystallographic orientations with respect to the substrate. Because the substrate acts as a seed crystal, the deposited film may lock into one or more crystallographic orientations with respect to the substrate crystal. If an epitaxial film is deposited on a substrate of the same composition, the process is called homoepitaxy; otherwise it is called heteroepitaxy. Epitaxy is used the manufacturing process of several semiconductor products, such as bipolar junction transistors, complementary metal-oxide-semiconductors and compound semiconductors.

Many evolution equations arising from epitaxy are nonlocal, higher order (fourth order or higher), and highly nonlinear, making their analysis rather complicated. It is indeed unclear whether solutions exist at all, even for short times. An advantage is however, that such systems are generally energy driven, hence such PDEs often exhibit a variational structure. My contribution involve providing analytical validation to several models, by proving the existence and regularity properties of solutions under suitable assumptions on the initial configuration.

1. Evolution equation from material sciences

Description of the problem. Discrete models to describe epitaxial growth with self-organization driven by misfit elasticity between film and substrate have been proposed by Duport, Politi and Villain [2], and Tersoff, Phang, Zhang and Lagally [7]. Continuum variants have been derived by Xiang [10], Xiang and E [11], Xu and Xiang [12]. In particular, in [10] it has been proven that the film's height profile h (which is assumed nonnegative and monotone) satisfies (upon inverting space coordinates) a fourth order equation of the form

$$h_t := -\left[H(h_x) + \left(h_x + \frac{1}{h_x}\right)h_{xx}\right]_{xx},$$

where H denotes the Hilbert transform.

For the simplified one-dimensional evolution equation, in [1], Dal Maso, Fonseca and Leoni proved existence and regularity of a variational solution for a suitable antiderivative u of h. However, as the definition of variational solution in [1] is quite weak (and significantly weaker than the classic weak solution), almost no regularity in time on u was proven, and the regularity in time is always assumed on the test function w.

For the related $2+1$ dimensional model, derived by Xu and Xiang in [12], there is no result on the existence of solutions, even for the simplified axisymmetric case, where (in polar coordinates) the evolution equation reduces to

$$h_t = -\Delta\left[\nabla\cdot(-\hat{r} + |h_r|h_r) + L(h_r) - (\nabla\cdot\hat{r})\log|h_r| - \frac{h_{rr}}{h_r}\right]. \tag{1}$$

Here $\hat{r}$ denotes the unit vector, h denotes the surface height of the film, and L is a linear operator given by

$$L(h_r)(r) := \int_0^{+\infty}\left(\frac{K(m)}{\rho+r} + \frac{E(m)}{\rho-r}\right)h_r(\rho)d\rho, \qquad m := \frac{4\rho r}{(\rho+r)^2},$$

with

$$K(m) := \int_0^{\pi/2}\frac{1}{\sqrt{1-m\sin^2\theta}}d\theta, \qquad E(m) := \int_0^{\pi/2}\sqrt{1-m\sin^2\theta}d\theta.$$

denoting the complete elliptic integrals of the first and second kind.

In another model, to account for wetting effects, Tegalin and Spencer derived in [6] the evolution equation

$$h_t = \Delta[h - h^{-2} - \Delta h]. \tag{2}$$

Here h^{-2} is the "wetting" term. Again, to our best knowledge, no results on the existence of solutions are available.

Research results. In collaboration with Fonseca and Leoni, we improved (in [3]) regularity properties for antiderivatives u, and proved that, under suitable initial conditions, there exists u is weak solution in the classical sense.

In [5] and [4] we provided analytical validation for (1) and (2) respectively, by proving the global existence in time of a strong solution, under rather weak regularity properties on the initial datum. Other results about existence and regularity of solutions were obtained in collaboration with Yuan Gao, Jian-guo Liu and Xiangsheng Xu.

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