Coarsening dynamics of the convective Cahn-Hilliard equation and faceted crytal growth

The coarsening dynamics of a faceted *vicinal* crystalline surface growing into its melt by *attachment kinetics* is considered. The convective Cahn-Hilliard equation ($\mathcal{CCH}$) is derived as a small amplitude expansion of such surface evolutions restricted to 1-D morphologies. It takes the form

$$q_t - \varepsilon q q_x = \left(\hat{W}'(q) - q_{xx}\right)_{xx}, \qquad (\mathcal{CCH})$$

where the local surface slope $q(x,t)$ serves as the order parameter, subscripts denote partial derivative with respect to time t and space x respectively, and $'$ denotes the q-derivative. The *effective free energy* $\hat{W}(q)$ takes the form of a symmetric *double well* with minima at $q = \pm 1$, thereby capturing the anisotropy of the crystal surface energy. Also, the dimensionless small parameter ε multiplying the convective term qq_x is a dimensionless measure of the growth strength.

A *sharp interface* theory for $\mathcal{CCH}$ is derived through a matched asymptotic analysis. The theory predicts a nearest neighbor interaction between two non-symetrically related phase boundaries (*kink* and *anti-kink*), whose characteristic separation $\mathcal{L}_{\mathcal{M}}$ grows as coalescing kink/anti-kinks annihilate one another. Theoretical predictions on the resulting (skew-symetric) coarsening dynamical system $\mathcal{CDS}$ include

- The characteristic length $\mathcal{L}_{\mathcal{M}} \sim t^{1/2}$, provided $\mathcal{L}_{\mathcal{M}}$ is appropriately small with respect to the *Peclet* length scale $\mathcal{L}_{\mathcal{P}}$.
- Binary coalescence of phase boundaries is impossible
- Ternary coalescence may only occur through the *kink-ternary* interaction; two kinks meet an anti-kink resulting in a kink.

Direct numerical simulations performed on both $\mathcal{CDS}$ and $\mathcal{CCH}$ confirm each of these predictions.

Last, a linear stability analysis of $\mathcal{CDS}$ identifies a *pinching* mechanism as the dominant instability, which in turn leads to kink-ternaries. We propose a self-similar period-doubling *pinch ansatz* as a model for the coarsening process, from which an analytical coarsening law for the characteristic length scale $\mathcal{L}_{\mathcal{M}}$ emerges. It predicts both the scaling constant c of the $t^{1/2}$ regime, i.e., $\mathcal{L}_{\mathcal{M}} = c\ t^{1/2}$, as well as the crossover to logarithmically slow coarsening as $\mathcal{L}_{\mathcal{M}}$ crosses $\mathcal{L}_{\mathcal{P}}$. Our analytical coarsening law stands in good qualitative agreement with large scale numerical simulations that have been performed on $\mathcal{CCH}$.

In part, joint work with Felix Otto and Stephen H. Davis.