Minimizers of an Energy Modelling Nanoparticle-Polymer Blends

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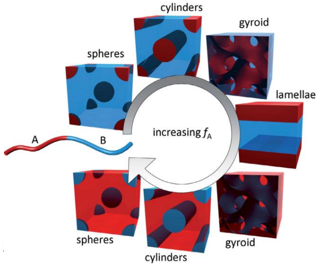
Diblock Copolymers

Diffuse-interface energy (Ohta-Kawasaki) passes to a sharp-interface model, a nonlocal isoperimetric problem (NLIP). In a sharp-interface limit, minimizers form phase domains, whose geometries depend on the volume fraction of the monomers and the strength of the nonlocal interactions.



f_A denotes the volume fraction of A-type monomers.

Extensive literature: Acerbi-Fusco-Morini, Alberti-Choksi-Otto, Bonacini-Cristoferi, Choksi-Glasner, Choksi-Peletier, Choksi-Ren, Choksi-Sternberg, Goldman-Muratov-Serfaty, Knüpfer-Muratov, Lu-Otto, Muratov, Ren-Wei, Shirokoff-Choksi-Nave, Sternberg-Topalaglu.

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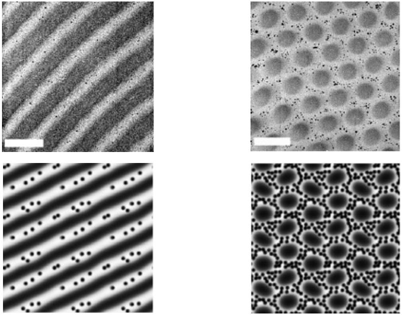
Study by the research group of Fredrickson: first column shows **low-density**, *second column shows* **high-density** *of nanoparticles.*



The Model – An Extension of Ohta–Kawasaki

Ginzburg-Qiu-Balacz, Polymer 43, (2002) 461-466

$$\begin{aligned} \mathrm{E}_{\epsilon,\gamma,\eta,m,r,u_p,N}(u;\mathbf{x}) := & \boxed{\frac{3\epsilon}{8}\int_{\mathbb{T}^n}|\nabla u|^2\,dx + \frac{3}{16\epsilon}\int_{\mathbb{T}^n}(u^2-1)^2\,dx} \\ & + \boxed{\frac{\gamma}{2}\int_{\mathbb{T}^n}\int_{\mathbb{T}^n} G(x,y)(u(x)-m)(u(y)-m)\,dxdy} \\ & + \eta\int_{\mathbb{T}^n}\sum_{i=1}^{N} V(|x-x_i|)(u-u_p)^2\,dx. \end{aligned}$$

The first three terms are Ohta-Kawasaki:

$u \in H^1(\mathbb{T}^n)$ is the phase parameter, ϵ=thickness of the phase transition.

$m \in (-1,1)$ determines the volume fraction of polymers: $m = \int_{\mathbb{T}^n} u(x)\,dx$.

γ=strength of the bond between phases, $G(x,y)$ denotes the Green's function on $\mathbb{T}^n$.

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The last term models nanoparticle-polymer interactions:

- $\mathbf{x} \in (\mathbb{T}^n)^N$ denotes the centers of N-many nanoparticles where each particle is a ball of radius r, $B(x_i, r)$.
- V=rapidly decreasing *(compactly supported)* repulsive potential.
- $u_p \in [-1, 1]$=nanoparticle preference towards polymer phases;
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We assume the nanoparticle locations $\mathbf{x} = (x_i)_{n=1,\dots,N}$ are fixed.

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\mathrm{E}_{\epsilon,\sigma}(u) := \frac{\epsilon}{2} \int_{\mathbb{T}^n} |\nabla u|^2 \, dx + \frac{1}{4\epsilon} \int_{\mathbb{T}^n} (u^2 - 1)^2 \, dx \\
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- Large number of nanoparticles, but small volume fraction:

$$N_\epsilon \to \infty, \ \text{ but } \ N_\epsilon r_\epsilon^n \to 0$$

- Assume the nanoparticles converge to a fixed distribution, $\mu \in \mathscr{P}_{\mathrm{ac}}(\mathbb{T}^n)$ representing a limiting nanoparticle density measure:

$$N_\epsilon \, r_\epsilon^n \sum_{i=1}^{N_\epsilon} \int_{B(x_i, r_\epsilon)} V(|x - x_i|/r_\epsilon)(u - 1)^2 \, dx \rightharpoonup \mu$$

Sharp Interface Limit

We first prove Γ-convergence of $\mathsf{E}_{\epsilon,\sigma}$ to the sharp interface energy,

$$\mathsf{E}_{\mu,\sigma}(u) := \frac{1}{2}\int_{\mathbb{T}^n} |\nabla u| + \sigma \int_{\mathbb{T}^n} (u(x)-1)^2 \, d\mu(x) + \frac{\gamma}{2}\int_{\mathbb{T}^n}\int_{\mathbb{T}^n} G(x,y)(u(x)-m)(u(y)-m)\, dxdy$$

with $u \in BV(\mathbb{T}^2; \{-1,1\})$, and where $\mu \in \mathscr{P}_{\mathrm{ac}}(\mathbb{T}^n)$ represents the limiting nanoparticle density measure.

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Notes on the Γ-limit:

- For the lower bound note that $\{u = 1\}$ and $\{u = 1\}^c$ are continuity sets of the measure μ.
- For the upper bound use the recovery sequence constructed by Sternberg for the perimeter. Combined with the weak-* convergence of the potentials to μ we get the upper bound.

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- The nonlocal term is treated as a continuous perturbation of the perimeter.

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We now restrict our attention to the **perimeter** *and* **penalization** *terms, and neglect the nonlocal interactions,* $\gamma = 0$ *in* $\mathsf{E}_{\mu,\sigma,\gamma}$.

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For $\rho \in L^1(\mathbb{T}^n)$ = density of $\mu \in \mathscr{P}_{\mathrm{ac}}(\mathbb{T}^n)$, minimization of $\mathsf{E}_{\mu,\sigma}$ is a geometric problem:

$$\text{minimize} \qquad \mathsf{E}_\sigma(\Omega) = \mathrm{Per}_{\mathbb{T}^n}(\Omega) + \sigma \int_{\Omega^c} \rho(x)\, dx$$

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Similar in the spirit to finding **minimal boundaries** with respect to an **obstacle set**: minimize perimeter of Ω so that an obstacle set is $L \subset \Omega$. (**Note:** no mass constraint.)

Barozzi-Massari, Barozzi-Tamanini, Brézis-Kinderlehrer, Giusti, S. Rigot, etc.

Properties of Local Minimizers

Proposition (Regularity of Phase Boundaries)

If $\rho \in L^\infty(\mathbb{T}^n)$ then $\partial^*\Omega$ is of class $C^{1,\alpha}$ for some $\alpha \in (0,1)$.

Idea: Control the excess-like quantity: $\mathrm{Per}_{B_R(x_0)}(\Omega) - \mathrm{Per}_{B_R(x_0)}(\widetilde{\Omega}) \leqslant C\,R^n$ where $\widetilde{\Omega}$ minimizes perimeter in $B_R(x_0)$. *See: Tamanini; Rigot*

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The effect of the nanoparticle density ρ is to change the curvature of the phase boundary $\partial\Omega$:

Proposition (First Variation)

If $\rho \in C^1(\mathbb{T}^n)$ then

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- This follows by adapting the calculations by Choksi-Sternberg.
- The equations are local on $\partial\Omega$, so if ρ is piecewise C^1 the curvature condition holds piecewise.

A special case: uniform nanoparticle density in a ball

Assume $\rho = \omega_n^{-1} r^{-n} \chi_{B_r}$ with $\omega_n r^n > m$. Then

$$\mathrm{E}_\sigma(\Omega) = \mathrm{Per}_{\mathbb{T}^n}(\Omega) + \sigma \left(1 - \frac{|\Omega \cap B_r|}{\omega_n r^n}\right)$$

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$$(n-1)\, H(x) = \lambda \quad \text{for } x \in \partial\Omega \cap \mathrm{int}\, B_r^c,$$

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That is, critical $\Omega \subset \mathbb{T}^2$ consist of pieces of constant mean curvature hypersurfaces, glued together in a $C^{1,\alpha}$ fashion. For $\sigma > 0$, the mean curvature is strictly larger inside the nanoparticle region B_r than it is outside.

An Example in 2-Dimensions

Recall: $\mathrm{E}_\sigma(\Omega) = \mathrm{Per}_{\mathbb{T}^n}(\Omega) + \sigma \int_{\Omega^c} \rho(x)\, dx$, $|\Omega| = m$.

Setup: $\mathbb{T}^2 = [-1/2, 1/2) \times [1/2, 1/2)$, with $m \in [1/2, 1 - 1/\pi)$

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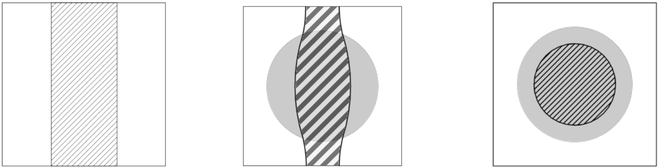
- Lamellar stripes must intersect nanoparticle set B_r, and disks B_R with area m lie inside B_r.
- For $\sigma = 0$ lamellar is the winner **but** as soon as we turn on $\sigma > 0$ lamellar is not even a critical point. **Regularity** implies that $\partial\Omega$ is $C^{1,\alpha}$. **Criticality** implies that $H_{\text{inside}} > H_{\text{outside}}$ and they are constant.



$\sigma = 0$ $\qquad$ $\sigma > 0$ small? $\qquad$ $\sigma > 0$ large?

What Other Patterns Are Possible?

Proposition

If Ω *minimizes* E_σ *then*

- *if* Ω *is contractible in* $\mathbb{T}^2$ *then* $A = B_R$ *with* $R = \sqrt{m/\pi}$*;*
- Ω^c *cannot be contractible in* $\mathbb{T}^2$*.*

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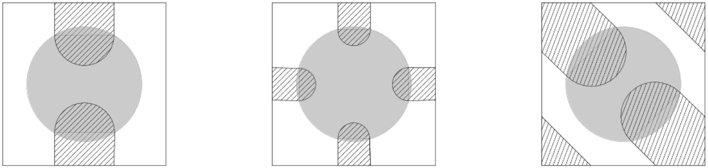
Criticality implies that $\partial\Omega$ is a union of arcs of circles and lines. **Regularity** implies that components of $\partial\Omega$ meet tangentially on ∂B_r. Recall **criticality** conditions:

$$\begin{aligned} H(x) &= \lambda \quad \text{for } x \in \partial\Omega \cap \operatorname{int} B_r^c, \\ H(x) &= \lambda + \frac{\sigma}{2\pi r^2} \quad \text{for } x \in \partial\Omega \cap \operatorname{int} B_r. \end{aligned}$$

The Lagrange multiplier is **either** $\lambda = 0$ or $\lambda < 0$. If $\lambda > 0$ then $\partial\Omega$ consist of positively curved arcs of circles which is **not** possible

Case 1: ($\lambda = 0$) $\partial\Omega$ = arcs of circles inside B_r and straight lines outside B_r. We get **band-aid** patterns. Stationary but not global minimizers for any $\sigma > 0$.



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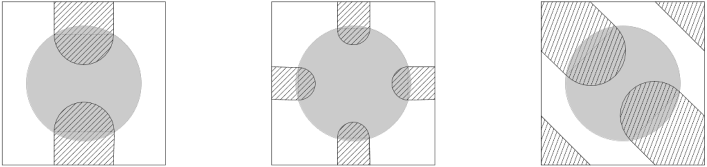
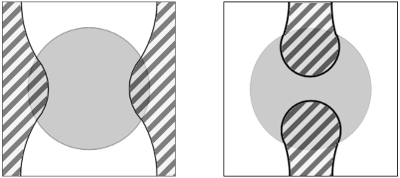
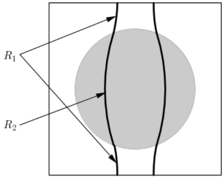


Case 2: ($\lambda < 0$) **Concave/convex strips**. $\partial\Omega$ consists of arcs of circles inside and outside of B_r: negatively curved outside of B_r and positively curved inside of B_r.



First pattern is unlikely to be a minimizer as the penalization term will be large for $\sigma > 0$. The second pattern is **not** a minimizer since it is contractible.

For sufficiently small $\sigma > 0$, **concave**/**convex** solutions exist (graphs over the lamellar stripe!)



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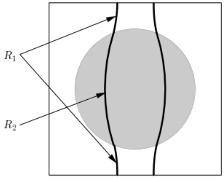

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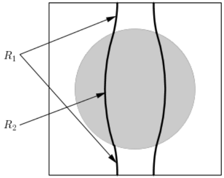

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Proposition

If Ω is a minimizer then $R_2 > r$ and $R_1 > 1/2 - r$. In particular, the convex-concave pattern can exist only if

$$\sigma = 2\pi r^2 \left(\frac{1}{R_1} + \frac{1}{R_2} \right) < \frac{2\pi r}{1 - 2r}.$$

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There exists $\sigma_0 = \sigma_0(m, r)$ *such that for all* $\sigma > \sigma_0$ *the set* $B_R \subset B_r$ *with* $R = \sqrt{m/\pi}$ *is the global minimizer of* E_σ.

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- Suppose Ω is a global minimizer which is not $B_R \subset B_r$. Then $\Omega \cap B_r \neq \emptyset$.

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- Compare the energy of Ω to $B_R \subset B_r$:

$$\mathrm{E}_\sigma(\Omega) - \mathrm{E}_\sigma(B_R) \geqslant (2 - 2\pi R) + \sigma \left(\frac{R^2}{r^2} - \frac{|\Omega \cap B_r|}{\pi\, r^2} \right) > 0$$

if

$$\sigma > \max\left\{ \sigma_1,\ \frac{4r^2(\pi\, R - 2)}{R^2} \right\} =: \sigma_0(m, r).$$

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- At the diffuse level, can we also minimize over the location of nanoparticles?

Thank you for your attention