Partial localisation in a variational model for diblock copolymer-homopolymer blends - summary (Yves van Gennip)

In this thesis we study pattern formation in a variational model for diblock copolymer-homopolymer blends. The goal of this research is to produce an understanding of the mathematical properties of the model that lead to pattern formation, develop or extend mathematical methods to investigate these properties and provide more information about the patterns themselves.

A diblock copolymer molecule consists of two polymer molecules of different type which are covalently bonded together. When both polymers are of immiscible types, they will want to separate at low temperatures. However, the covalent bond imposes a constraint on the length of separation they can achieve. This phenomenon, which is called microphase separation, leads to pattern formation in diblock copolymer melts. In such a melt at low temperatures regions will form of high concentration of one of the polymer types and low concentration of the other and regions where the roles are reversed. These regions form patterns. For example, both regions can alternate in a lamellar fashion or spherically shaped regions of one type can be included in a background of the other type.

The lamellar pattern is an example of a spatially extended pattern, since the whole domain is filled with lamellae. The spherical pattern on the other hand is a localised pattern, since the spherical regions are structures which are small, localised in all directions. In the current research the main interest is in the formation of so called partially localised patterns: structures which extend in some directions and are small in others. An example of a pattern like this in nature is the membrane that surrounds a living cell. It is small in the direction perpendicular to the membrane and extended in the other directions. There are strong indications that these kind of patterns do not emerge in diblock copolymer melts, which is why the attention in this thesis is directed to a model of an extension of that system: diblock copolymer-homopolymer blends.

In such blends a homopolymer, i.e. a polymer consisting of one monomer type, is added to the diblock copolymer melt. If this homopolymer is of a type which does not mix with the polymer types in the diblock copolymer, an extra repelling force will emerge in the system, separating the homopolymer from the diblock copolymer. The competition between this repelling force, the internal repulsion in the diblock copolymer and the covalent bonding in the copolymer will lead to separation on two scales: on a macroscale the homopolymer and diblock copolymer will separate and on a microscale the microphase separation of the diblock copolymer will be seen. This multiscale behaviour opens up the possibility of partially localised structures.

The mathematical model used to describe these blends is variational in nature. This means a functional is given which assigns an energy value to each possible pattern. Minimisers of this functional then describe the patterns that are seen in the physical system.

Finding explicit minimisers of the functional is too hard a problem in general, which is why we follow various routes to better understand the model. In the simplified context of a one-dimensional setting we completely describe minimisers of the energy. In higher dimensions however the problem becomes significantly more complex because of the increase in morphological freedom patterns have. We compute bounds on the energy of minimisers using a result which tells us what the energetic consequences are of extending a lower dimensional pattern in a straightforward manner to a higher dimensional structure. We also do a stability analysis on two-dimensional mono- and bilayers, structures which are believed to be energetically favourable, if not global minimisers. This analysis shows a delicate dependence of stability on the surface tension parameters in the model.

We also study a related energy functional defined on curves in two dimensions to investigate some specific properties of the original model in a setting tailored to the needs of partially localised structures.

This thesis provides many new insights into the blend model, which has not undergone much mathematical scrutiny before, and improves our understanding of how partially localised structures emerge in mathematical models that carry a relevance for physical systems.