

Multiscale topology optimization for self-assembling diblock copolymers

Nicola Parolini*, Francesco Regazzoni and Marco Verani

MOX, Dipartimento di Matematica
Politecnico di Milano
Piazza Leonardo da Vinci 32, Milano, Italia
e-mail: nicola.parolini@polimi.it, web page: <http://mox.polimi.it/parolini>

ABSTRACT

Diblock copolymers are linear chain molecules made of two subchains joined covalently to each other which exhibit interesting physical properties. When binary mixtures of diblock copolymers undergo a critical temperature, they spontaneously arrange in regular and periodic structures of some nanometers characteristic length. This self-assembling process is described by a nonlocal version of the Cahn-Hilliard equation, the Cahn-Hilliard-Oono equation, that can be numerically solved to predict and control pattern formation.

In this talk we propose a two-scales topology optimization approach for the solution of the problem: at the microscale Cahn-Hilliard-Oono equation rules the pattern formation, while at the macroscale the equilibrium configuration of the elastic body is determined by the linear elasticity equation. Homogenization theory is employed to link the two scales. By controlling the parameters that modulate the diblock copolymers phase separation, we locally optimize the typology and orientation of these patterns, in order to maximize the elastic response of a macroscopic body. At the same time the shape of the body is optimized, under a total mass constraint.

The numerical solution of the PDEs governing the two scales, as well as of those associated with the homogenization procedure, is based on the finite elements method (FEM). To tackle discontinuities in the state plane of diblock patterns, a multi-material problem is formulated and a new algorithm that generalizes the Optimality Conditions method for topology optimization to the multi-material case is proposed. A detailed derivation of the method together with a set of numerical simulations assessing its performances can be found in [1].

REFERENCES

- [1] Regazzoni, F., Parolini, N. and Verani, M., Topology optimization of multiple anisotropic materials, with application to self-assembling diblock copolymers. *Comput. Methods Appl. Mech. Eng.* (2018) **338**:562–596.