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Perspective: Evolutionary Design of Granular Media and Block Copolymer Patterns

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Scientific Achievement

In this invited perspective we review newly emerging approaches for the optimized design of materials under conditions both near and far from equilibrium. The creation of new materials "by design" is a process that starts from desired materials properties and proceeds to identify requirements for the constituent components. Such process is challenging because it inverts the typical modeling approach, which starts from given micro-level components to predict macro-level properties. We describe how to tackle this inverse problem using concepts from evolutionary computation. These concepts have widespread applicability and open up new opportunities for design as well as discovery. We show how they can be applied to design tasks involving two very different classes of soft materials, shape-optimized granular media and nanopatterned block copolymer thin films.

Significance

The ideas and algorithms outlined in this perspective are precursors to what we think could be a paradigm shift in how soft matter is designed, one that would enable cycles of design, synthesis and characterization that, for the first time, occur truly co-currently, with potentially extraordinary increases in efficiency and productivity. The approaches discussed are not limited to equilibrium conditions. They are extremely effective also far from equilibrium, where much less is known about materials behavior and design. Not only can the materials processing pathway be included explicitly, but identifying the most suitable pathway can become the actual design target. This paves the way for macromolecular assembly processes that lead predictably and reliably towards useful, non-equilibrium morphologies. We posit that it is only by relying on such design approaches that the materials science community will be able to harness the full spectrum of structure and function that soft materials have to offer.

Citation

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