Scaling up polymer blobs

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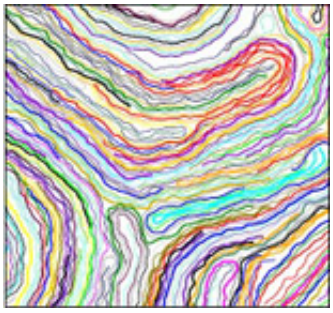

Scientists use simulations to test the limits of their object of study—in this case thin films of polymers—to extremes of scale. In a study about to be published in the *European Physical Journal E*, Nava Schulmann, a researcher at Strasbourg University, France, and colleagues use a well-known model capable of providing information on heat and mechanical energy exchange between these polymer chains. They found that polymer blends confined to ultrathin two-dimensional films displayed enhanced compatibility. This was made possible by simulations using a fairly standard model, which is simple enough to allow the efficient computation of dense large-chain systems.

The authors focused on making simulations of self-avoiding and highly flexible polymer chains without chain intersections. To do so, they varied the level of polymer density, as well as their chain length, while using numerical methods to arrive at a universal view of polymer

behaviour.

Thanks to molecular dynamics and so-called Monte Carlo simulations, they confirmed that such polymers adopt a scaling behaviour following a power law as a function of density and chain length. This scaling behaviour applies, for example, to polymer pressure and, hence, polymer compressibility. French Nobel laureate Pierre-Giles de Gennes predicted this property in his so-called blob picture approach. Accordingly, a polymer chain is akin to a succession of blobs, like beads in a necklace.

Schulmann and colleagues focused on a regime relevant for applications, referred to as a semi-dilute regime. There, scaling occurs more universally as long as the initial blob size is well defined. Understanding the limit of a system of long chains can currently only be realised in simulations of simplified models. However, the authors hope their findings will facilitate the work of polymer experimentalists.[2]

More information: N. Schulmann, H. Meyer, P. Polińska, J. Baschnagel, and J.P. Wittmer, Strictly two-dimensional self-avoiding walks: Thermodynamic properties revisited, (2012) *European Physical Journal E* 35:93 DOI 10.1140/epje/i2012-12093-x

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