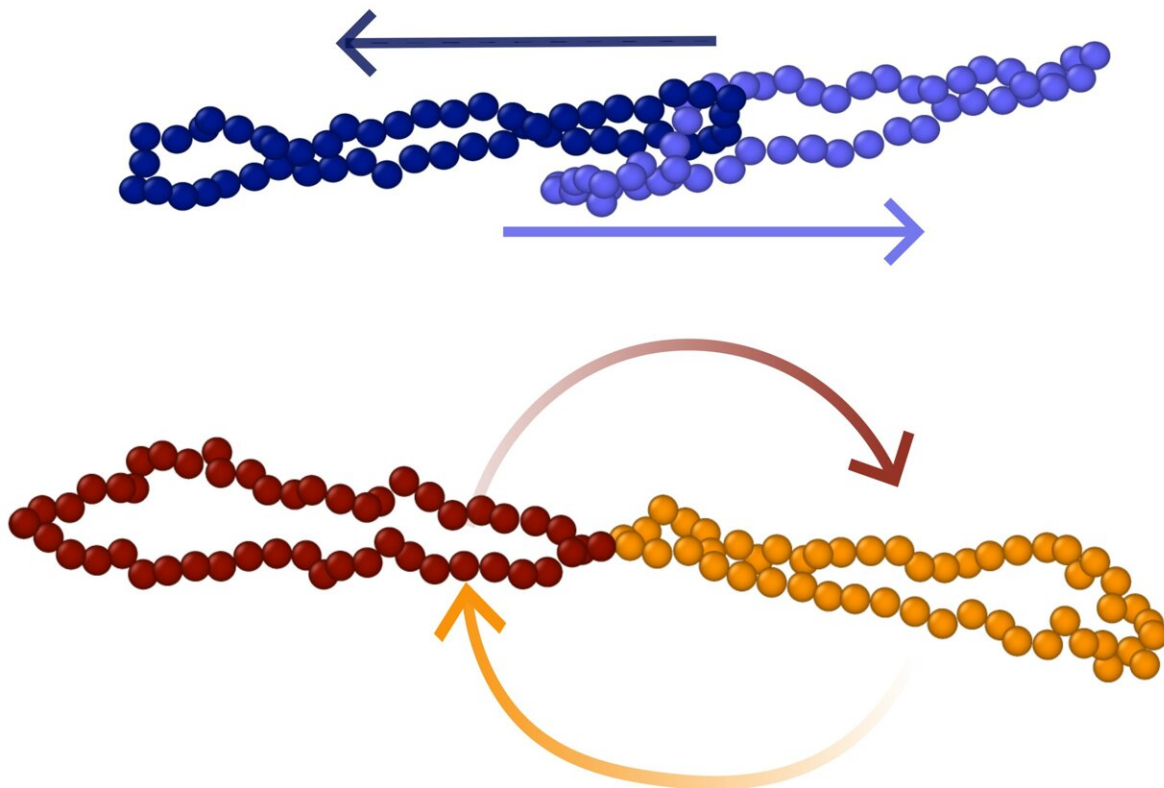


Physics of complex fluids: Ring polymers show unexpected motion patterns under shear

April 4 2024



Schematic of poly[2]catenane slip tumbling and bonded ring gradient tumbling.
Credit: Reyhaneh A. Farimani

The shearing of fluids—meaning the sliding of fluid layers over each other under shear forces—is an important concept in nature and in rheology, the science that studies the flow behavior of matter, including liquids and soft solids. Shear forces are lateral forces applied parallel to a material, inducing deformation or slippage between its layers.

Fluid shear experiments allow the characterization of important rheological properties such as viscosity (resistance to deformation or flow) and thixotropy (decrease in viscosity under the influence of shear), which are important in applications ranging from industrial processes to medicine. Studies on the shear behavior of viscoelastic fluids created by introducing polymers into Newtonian fluids have already been conducted in recent years.

However, a novel approach in the current research involves the consideration of [polymer](#) topology—the [spatial arrangement](#) and structure of molecules—by using [ring](#) polymers. Ring polymers are macromolecules composed of repeating units, forming closed loops without free ends.

A matter of linking

First author Reyhaneh Farimani explains, "For our computer simulation experiments under shear, we considered two similar types of connected ring pairs: One in which the linkage is chemical, called bonded rings (BRs), and one in which the linkage is mechanical via a Hopf link, called polycatenanes (PCs)."

Special emphasis was placed on taking into account hydrodynamic interactions through appropriate simulation techniques, which proved to be crucial since a delicate interplay between fluctuating hydrodynamics and topology governs the emerging patterns.

The results were surprising: On the one hand, the response of the two components, BRs, and PCs, was very different from each other—and on the other hand, it was clearly different from that of various other polymer types, such as linear, star, or branched. In particular, the dominant dynamic pattern in other polymers under shear ("vorticity tumbling") is either suppressed (BRs) or virtually absent (PCs) in these topologically modified polymers.

Unexpected types of tumbling

"What we discovered," says Christos Likos, co-author of the study, "are completely unexpected dynamic patterns in both ring polymer types, which we call gradient-tumbling and slip-tumbling." Due to an interplay between hydrodynamics and ring topology, the BR molecules tumble around the gradient direction, which is perpendicular to the vorticity and flow axes. BRs are found to be in a continuous gradient-tumbling motion under shear.

On the contrary, PCs become thin, orient themselves close to the flow axis, and maintain a fixed, stretched, and non-tumbling conformation under shear. Instead, due to their peculiar form of mechanical linkage, PCs exhibit intermittent dynamics, with occasional exchange of the two rings as they slip through each other, a pattern the authors of the paper call slip-tumbling.

These unexpected modes of motion, which bear unique signatures of the topologies of the polymer compounds, underscore the importance of the interplay between hydrodynamics and polymer architecture. In fact, the researchers found in their simulations that when the backflow effects are artificially eliminated, the differences between BRs and PCs disappear.

These dynamical modes also have a noticeable effect on the mechanical properties of the solution since BRs release internal stresses by tumbling,

whereas PCs store stresses permanently, resulting in a much higher viscosity in the latter case. This leads to the hypothesis that the different tumbling motions and structures of PCs and BRs could influence the shear viscosity—a fluid's resistance to flow under shear reflecting its internal friction and ability to deform—of highly concentrated solutions or polymer melts of these molecules.

Further experimental and theoretical studies are needed to test this hypothesis. The current study was conducted by a scientific cooperation between the University of Vienna, the Sharif University of Technology in Iran, and the International School of Advanced Studies (SISSA) in Italy.

The work is [published](#) in the journal *Physical Review Letters*.

More information: Reyhaneh A. Farimani et al, Effects of Linking Topology on the Shear Response of Connected Ring Polymers: Catenanes and Bonded Rings Flow Differently, *Physical Review Letters* (2024). [DOI: 10.1103/PhysRevLett.132.148101](https://doi.org/10.1103/PhysRevLett.132.148101)

Provided by University of Vienna

Citation: Physics of complex fluids: Ring polymers show unexpected motion patterns under shear (2024, April 4) retrieved 2 May 2024 from <https://phys.org/news/2024-04-physics-complex-fluids-polymers-unexpected.html>

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